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MATHEMATICAL MODELLING

*A Tool for Problem Solving in Engineering,
Physical, Biological and Social Sciences*

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PERGAMON PRESS

Member of Maxwell Macmillan Pergamon Publishing Corporation

OXFORD · NEW YORK · BEIJING · FRANKFURT
SÃO PAULO · SYDNEY · TOKYO · TORONTO

U.K.	Pergamon Press plc, Headington Hill Hall, Oxford OX3 0BW, England
U.S.A.	Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, New York 10523, U.S.A.
PEOPLE'S REPUBLIC OF CHINA	Pergamon Press, Room 4037, Qianmen Hotel, Beijing, People's Republic of China
FEDERAL REPUBLIC OF GERMANY	Pergamon Press GmbH, Hammerweg 6, D-6242 Kronberg, Federal Republic of Germany
BRAZIL	Pergamon Editora Ltda, Rua Eça de Queiros, 346, CEP 04011, Paraiso, São Paulo, Brazil
AUSTRALIA	Pergamon Press Australia Pty Ltd, P.O. Box 544, Potts Point, N.S.W. 2011, Australia
JAPAN	Pergamon Press, 5th Floor, Matsuka Central Building, 1-7-1 Nishishinjuku, Shinjuku-ku, Tokyo 160, Japan
CANADA	Pergamon Press Canada Ltd., Suite No. 271, 253 College Street, Toronto, Ontario, Canada M5T 1R5

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First edition 1990

Library of Congress Cataloging-in-Publication Data

Murthy, D. N. P.
Mathematical modelling: a tool for problem solving in
engineering, physical, biological, and social sciences/D. N. P.
Murthy, N. W. Page & E. Y. Rodin. — 1st ed.
p. cm. — (International series in modern applied
mathematics and computer science)
1. Mathematical models. I. Page, N. W. II. Rodin, E. Y.
III. Title. IV. Series.
QA401.M87 1989 511'.8—dc20 89-16246

British Library Cataloguing in Publication Data

Murthy, D. N. P.
Mathematical modelling.
1. Mathematical models.
I. Title II. Page, N. W. III. Rodin, E. Y.
511'.8

ISBN 0-08-037244-9

Printed in Great Britain by BPCC Wheatons Ltd, Exeter

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Preface

Problems in the real world arise in many contexts. It could be:

- (i) to gain new understanding about some phenomena, for example how does a forest fire spread;
- (ii) to obtain the response behaviour of a system, such as the flight of a rocket;
- (iii) to design a complicated piece of equipment like a thermal power station;
- or
- (iv) to optimize some performance measure such as profits of a company.

Although problem solving has been practised for a very long time, the use of mathematics as a very effective tool in problem solving has gained prominence in the last 50 years, mainly due to the rapid developments in computing.

The critical step in the use of mathematics for solving real-world problems is the building of a suitable mathematical model. The importance of this is recognized in the fact that the past 20 years has seen the appearance of a large number of books on mathematical models and modelling, and several journals devoted to the topic.

In the literature, models are often presented in their final, neat and elegant form. In reality there are many steps, choices and iterative processes that a modeller goes through in reaching a satisfactory model. These features are usually hidden, and hence the beginner fails to see them. Each step in the modelling process requires an understanding of a variety of concepts and techniques blended with a combination of critical and creative thinking, intuition and foresight, and decision making. This makes model building both a science and an art.

This book advocates a novel approach to the teaching of the building process for mathematical models. The essential features of the approach are its scope, an emphasis on the art as well as the science aspects, and the development of a self-learning process by the student.

The art aspect of modelling is difficult to teach in any formal sense. We have adopted a "learning through doing" approach somewhat akin to studio activities in, say, architecture. In this self-learning activity the instructor plays

a critical role in guiding the student to appreciate the art aspect in an open and constructively critical environment. In addition to developing the various thinking and decision making skills, this format develops confidence in the student to solve new and unfamiliar problems.

A special difficulty in the teaching of the science aspect is the breadth and depth of material needed for model building. The approach we have taken is as follows. We develop an overview of the modelling process to identify the different topics needed for model building, highlight the basic concepts and relevance of each topic and finally guide the student to learn the details through a self-learning approach by providing a rich bibliography. This not only achieves a sensible resolution of the conflict between breadth and depth but, more importantly, avoids the familiar trap where the student fails to differentiate the trees from the woods.

In summary, the aims of the book are to develop in the student:

- (i) an appreciation of the total view of the modelling process from its logical starting point to the final point which yields the desired solution to the problem of interest;
- (ii) an understanding of the framework to carry out the modelling process;
- (iii) an understanding of the role and significance of the different topics relevant to the modelling process;
- (iv) an appreciation of the art and the science aspects of mathematical modelling;
- (v) the need for active self-learning.

In addition, it aims to help the instructor discharge his role as a guide.

The book is structured into the following three parts:

Part I Methodology and Tools

Part II Case Studies

Part III Supplementary Material

Part I consists of 13 chapters, and deals with the concepts and techniques needed for modelling. An outline of the different chapters is given in Chapter 1. Part II consists of three detailed case studies which bring all the material covered in Part I together in the context of model building. Part III consists of two chapters. The first deals with a large number of real-world problems suited for mathematical modelling which are meant for use as modelling exercises. The second is primarily meant for the instructor as a source for supplementary material. It contains a list of books on mathematical models and modelling, and a comprehensive list of articles on models, modelling and the teaching of modelling.

Different levels of mathematical background are needed to appreciate and understand the different topics covered in Part I. It is doubtful if any

undergraduate programme would provide the ideal mathematical background required. As a result, many topics will be new to the student. A word of caution is appropriate at this stage. Our approach to teaching mathematical modelling requires a broad overview of the modelling process which would be obscured to some extent if all details were provided. Consequently, the instructor will need to give the student an intuitive feel for any topic with which the student is unfamiliar, and should encourage the student to embark on a self-learning venture. Such a venture will not only cover any deficiency in the student's background but, more importantly, it will develop the self-learning and other skills needed for mathematical modelling. Notes at the end of each chapter give suitable references as starting points for such ventures.

The book can be used as a text for teaching mathematical modelling at two different levels in an undergraduate programme. At the first level (suited for the 2nd or 3rd year of an undergraduate programme in science or engineering) it can be used for an introductory course on deterministic modelling based on the following chapter sequence:

Chapters 1–2–3–4–5–6–10 (part)–12 (part)–13.

At the second level (suited for the 3rd or 4th year of an undergraduate programme in science or engineering) it can be used for an introductory course on stochastic modelling based on the following chapter sequence:

Chapters 1–2–3–4–7–8–9–10–11–12–13.

At the postgraduate level this book can be used with Part III as the starting point and the student producing an end-product similar to that in Part II. This would require material from all earlier chapters, supplemented by additional material from the references at the end of each chapter.

It is impossible to acknowledge individually the authors of scores of publications on mathematical modelling, and the teaching of mathematical modelling, that have influenced the authors over their long period of interest in this topic. We have attempted to make our reference list as comprehensive as possible. Any omission is unintentional and the authors apologize for it.

Chapter 14 is heavily influenced by the work of Dr. Bailey. Table 14.1 and various parameter estimates are from his book *The Biomathematics of Malaria*, and we thank the publishers, Charles Griffin Company, for their permission to use them. Also we thank the World Health Organization for their permission to reproduce Figures 14.1 and 14.3, and related equations from their *Bulletin*. Chapter 15 is based on a paper by Drs. Martens and Bell. We would like to thank them, and the American Society of Mechanical Engineers, for their permission to make extensive use of the material in our chapter. Section 2 of Chapter 18 is based on a paper which appeared in

Mathematical Modelling, and the authors thank Pergamon Press for their permission to use the material.

Many people read one or more chapters of earlier versions and gave helpful comments. In particular we would like to thank Drs. Peter Jacobs, Duncan Gilmore, Phil Diamond, Lou Westphal and Bill Daniel. The authors take full responsibility for the final version and any shortcomings. Istiana Djamaludin checked the reference lists with great care, and the authors are indebted to her for her services.

Special thanks are due to the typists who were involved in the various versions. In particular, our thanks to Joan Krendlinger, Judy Wheelan and Kathryn Lancaster for their efforts.

Finally, this book is dedicated to teachers all over the world who are involved in teaching mathematical modelling.

PART I

METHODOLOGY AND TOOLS

CHAPTER 1

Role of Mathematics in Problem Solving

1 Introduction

The use of mathematics in solving real-world problems (as distinct from artificial textbook problems) has become widespread in recent times. This is partly due to the use of the systems approach to problem solving, and to the increasing computational power of digital computers and computing methodology, both of which have made many more problems amenable to mathematical solution. There is hardly a branch of learning where mathematics and computing have not made an impact.

The steps involved in using mathematics to solve real-world problems are shown in Figure 1.1. The most crucial and important step is the satisfactory translation of the problem from the real physical world into a mathematical description. Once this is done, standard techniques of mathematical analysis can be used to obtain a solution to the problem. The validity of the solution depends on how well the mathematical description models the real world. The mathematical description is called a mathematical model, and the process of obtaining it is called mathematical modelling.

The use of mathematics is one of many approaches to solving real-world problems. Others include experimentation either with scaled physical models or with the real world directly. The mathematical approach has a number of advantages which can best be illustrated by considering a number of specific examples.

Example 1

What is the thrust level and duration necessary to ensure that a rocket reaches the moon? In this problem a solution based on an experimental programme involving rocket launches with different thrust-time histories is obviously unacceptable due to the cost and the uncertainty of success. Furthermore, the solution to this problem cannot be obtained using scale-model experiments. This problem lends itself to a mathematical treatment.

Example 2

What are the consequences of changes to the operation of an existing chemical plant? For safety and cost reasons it would be undesirable to carry out the changes on the plant itself without first

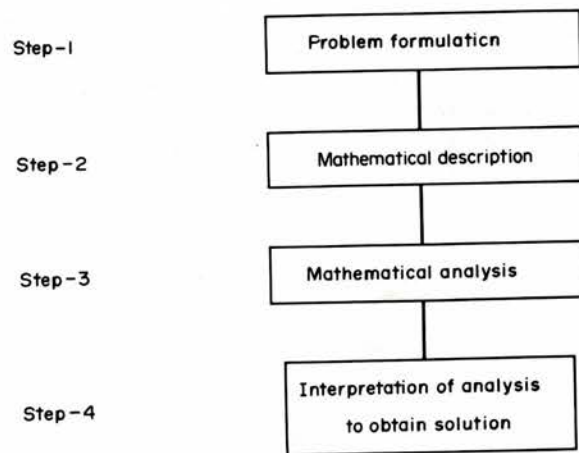


FIGURE 1.1 Problem solving using mathematics.

knowing the outcome. A scaled physical model could be used to obtain the desired information, but this would require special facilities. A mathematical approach would clearly be attractive here.

Example 3

What will be the growth in the number of airline passengers over the next 5 years? Forecasts of this nature are frequently needed for planning purposes. There is really no scientific alternative to a mathematical treatment for problems of this kind.

In this book we concentrate on the process of mathematical modelling. Our aim is to develop this process in a framework which highlights all aspects of the modelling process. Failure to understand and appreciate the relevance of these different aspects will result in the creation of a mathematical model which is of limited use in solving the real-world problem at hand.

In the remainder of this chapter we discuss the following topics:

- (i) nature of mathematical modelling,
- (ii) approach to the modelling process,
- (iii) an outline of the structure of the book.

2 The Nature of Mathematical Modelling

Mathematical modelling is the process by which a problem as it appears in the real world is interpreted and represented in terms of abstract symbols. This abstract description involving a mathematical formulation is called a mathematical model of the original problem. In this abstract form the problem is divorced from the real world and can be treated in mathematical terms only. In other words the underlying formulation may be viewed as a dummy, much like a tailor's dummy, and mathematical modelling as the process of clothing

the dummy in terms of the features of the real world. For example, a single mathematical formulation (dummy) may be appropriate for a number of physical problems with the mathematical symbols taking on different meanings (clothes) depending on the problem under consideration. Consider the following equation for one dependent variable (ϕ) in terms of two independent variables (x, t) and one parameter (α).

$$\partial\phi/\partial t = \alpha\partial^2\phi/\partial x^2$$

This single mathematical formulation can be used to describe a number of quite different problems. For example, if t represents time and x one spatial coordinate, then ϕ could be the temperature in a one-dimensional heat conduction problem, or species concentration in a one-dimensional diffusion problem.

In order to carry out a mathematical modelling exercise one requires an understanding of many different topics. Some topics are needed for dealing with the problem as it appears in the real world and others for dealing with the formulation belonging to the abstract world of mathematics. In addition, one needs skills to relate these two distinctly different worlds – the real world of the problem and the abstract world of the mathematical formulation.

Mathematical modelling is an *art* as well as a *science*. The science aspect deals with the topics needed to execute the various steps in the modelling process. Because no two problems are the same in the real world, features such as creativity, intuition and foresight also play an important role in the modelling process. These features constitute the art aspect of mathematical modelling. This makes mathematical modelling a very challenging, and at the same time a very demanding, activity. The science aspect can be appreciated in a passive learning mode, whereas the art aspect can be appreciated only by learning in an active mode – i.e. by building mathematical models and learning from experience.

Seldom does one obtain an adequate mathematical model at the first attempt for the problem under consideration. In general an iterative procedure is needed where improvements are progressively made until an adequate mathematical model is obtained. The art aspect of modelling is very important during this iterative phase.

3 Approach to the Modelling Process in this Book

Many different approaches have been advocated for learning the mathematical modelling process. This is reflected in the large number of books and journal articles that have appeared over the past decade on mathematical models and modelling, many of which are included in the references at the end of this chapter. A more comprehensive and annotated list is given in Chapter 17.

This book employs an approach, the aims of which are as follows:

- (1) The power of mathematical modelling as a tool for solving a wide variety of real-world problems is illustrated with many examples.
- (2) A universal and comprehensive framework is developed for model building. This framework identifies the main activities involved in model building.
- (3) The important features of each of the main activities involved in modelling are discussed separately. Their use is illustrated through a series of case studies in which mathematical models are built for selected real-world problems.
- (4) All the different activities are brought together to illustrate the modelling process in its totality by considering three case studies in depth.
- (5) In the spirit of learning by participation, a number of exercises are given for solution by the student with the purpose of developing mathematical modelling skills. These exercises consist of a number of real-world problems. A brief description is given of each, together with a short list of references.

An important feature of this approach is the extensive use of case studies to illustrate the various aspects of mathematical modelling. Twelve case studies have been used for this purpose. They have been chosen from a wide range of disciplines to encourage a broad understanding of the science and art aspects of modelling, and to demonstrate the universal nature of the modelling process.

4 The Systems Approach

The starting point in any problem-solving activity, whether it involves mathematical modelling or not, is to define clearly and unambiguously the problem to be solved. This aspect is discussed in Chapter 2 where the ideas are applied to the 12 case studies with a view to the subsequent development of mathematical models which will be used to obtain solutions.

As will be seen from Chapter 2, problems typified by the case studies considered are all different in some respect. For the purpose of developing a methodology for mathematical modelling, it is essential to develop a universal framework that facilitates a common approach to all problems. The "systems approach" offers such a framework in which problems are viewed as being embodied in a system. By viewing the problem in this framework the characteristics of the system important to the problem can be clearly identified. This is the first step towards the development of a mathematical model. This process of "system characterization" is treated in Chapter 3.

5 Mathematical Modelling and Structure of the Book

Once the system characterization is completed, the next step is the construction of the mathematical model. There are many different kinds of models, and

these are discussed in Chapter 4. A classification system for mathematical models is also given in that chapter, for the purpose of helping the reader make a better match between the system characterization and the mathematical formulation chosen for the model.

An overview of various mathematical formulations and examples of their application are given in Chapters 5 and 7. This broad overview is intended to provide the reader with a knowledge of the variety of mathematical formulations available for a particular modelling problem. Notes and references are provided at the end of each chapter to help the reader find detailed information about selected formulations. This format is an important feature of the approach to teaching mathematical modelling in this book, as it leads to a unique combination of both breadth and depth. Chapters 6, 8 and 9 give an overview of mathematical tools available for carrying out analysis to obtain solution to the problem under consideration. Chapters 10–13 deal with steps needed to establish model credibility and its usefulness to yield a meaningful solution to the problem in question. Here again the emphasis is on giving a broad overview, with notes and references provided to give access to more detailed information.

Chapters 3–12 cover separately the different topics needed for mathematical modelling. These topics are brought together in Chapters 14–16, where the modelling process is discussed in its totality and illustrated by detailed application to three case studies. For each case study the complete iterative process used to obtain an adequate model for the specified problem is presented.

Notes and References

The use of mathematics and computers for solving real-world problems is very widespread. There is hardly a branch of learning where mathematics and computers have not made an impact.

It is impossible to give a comprehensive list of books on the use of mathematics in different disciplines as it would run into hundreds. Instead, we give an illustrative sample: [1]–[4] deal with mathematics in biology and medicine; [5]–[8] deal with mathematics in social sciences; [9]–[12] deal with mathematics in physical sciences; [13]–[16] with mathematics in humanities, and [17] and [18] deal with mathematics in sports.

Two introductory-level books which illustrate the effectiveness of mathematics in solving a wide variety of problems are [19] and [20]. A large number of interesting articles, at a fairly introductory level, on the application of mathematics to solving a diverse range of real-world problems can be found in [21].

The activity of problem solving, though practised for a very long time, has received formal attention only over the past few decades. The number of books on problem solving is again fairly large, and [22]–[26] is a small sample. The

morphology of mathematical problem solving has received some attention and many alternative characterizations have been proposed. The one shown in Figure 1.1 is adequate for our purpose, and will form the basis for subsequent discussions.

Problem solving requires various types of thinking – creative, critical, deductive, inductive, scientific, intuitive, etc. Again, there are a large number of books dealing with different facets of this interesting topic. Items [27]–[30] form a small illustrative sample. It is recommended that advanced-level students in modelling read one or more of these, or similar, books.

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CHAPTER 2

Problem Definition: The Starting Point

1 Introduction

The problem that needs to be solved must be clearly defined before any mathematical modelling can commence. In problems drawn from the real world this is done by describing the context of the problem and then stating the problem within this context. In this chapter the process of problem definition is illustrated in 12 case studies. These case studies are based on real-world problems that will be used throughout the book to teach the modelling process. They will be repeatedly referred to in later chapters to illustrate different aspects of the mathematical modelling process.

2 Case Studies

The 12 case studies are labelled A–L. As discussed in Chapter 1, they have been deliberately chosen to cover a wide range of subject matter. Table 2.1 gives chapter and section numbers where each of the 12 case studies are used in the remainder of the book, to illustrate the role and significance of different topics in modelling.

Although it is not essential to read all the case studies, and to follow these throughout the book, a better understanding and appreciation of the underlying universal framework used to develop mathematical models is best achieved by studying a broad sample of the case studies.*

2.1 Case Study A (Weight Lifting)

In weight lifting competitions the lifters are grouped into seven different categories based on their body weights. There are two common lifting styles formalized in competition – jerk, in which the weight is lifted in two steps, one

*Those reading the book for the first time are advised to read Case Studies A, D, and E if they are interested in deterministic modelling, and Case Studies I and J if the interest is in stochastic modelling. In subsequent readings they are urged to read the remaining case studies.

TABLE 2.1 Section Index to Case Studies A–L

	Case Studies											
	A	B	C	D	E	F	G	H	I	J	K	L
Problem definition Chapter 2	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	2.10	2.11	2.12
System characterization Chapter 3	2.2 6.1	4.0 6.2	6.3	4.0 5.0 6.4	3.0 4.1 6.5	6.6	6.7	2.1 2.2 4.2 6.8	2.1 3.0 5.0 6.9	6.10	2.1 6.11	2.2 4.1 6.12
Mathematical models Chapter 4	—	—	—	—	4.0	—	—	—	—	—	—	—
Deterministic models Chapter 5	3.2	—	3.4	5.4	4.5 5.5 6.1 7.4	7.5	—	—	—	—	—	—
Stochastic models Chapter 7	—	4.2	—	—	—	—	5.3	—	6.7 8.4	4.4 8.5	6.5	7.4
Model analysis Chapter 6	—	—	5.3	4.2 4.4 7.4 7.6	6.2 7.2 8.5	8.2	—	—	—	—	—	—
Chapter 8	—	—	—	—	—	—	4.4	—	6.3 8.4	3.2 8.3	5.2	—
Simulation Chapter 9	—	—	—	5.3	2.3	—	—	—	—	—	3.3 5.7	—
Parameter estimation Chapter 10	3.5	—	—	2.2	3.6	—	4.8	—	4.5 4.7	4.2	—	4.9
Design of experiment Chapter 11	—	2.4	—	—	—	—	—	5.4	7.2	—	—	—
Validation Chapter 12	4.5	—	—	3.1	—	—	3.1 5.7	—	—	5.6	—	—

TABLE 2.2 Data for Case Study A: Weight Lifts for Different Weight Categories

Bodyweight class	Winning weights		
	Snap	Jerk	Total
Flyweight (52)*	105	137	242
Bantamweight (56)	117	145	262
Featherweight (60)	125	160	285
Lightweight (67.5)	135	172	307
Middleweight (75)	145	190	335
Light-heavyweight (82.5)	162	202	364
Middle-heavyweight (90)	170	212	382
Heavyweight (100)	175	225	400

*Mean body weight in kilograms for the class

taking it to chest height and the second taking it to full height; and snatch, in which the weight is lifted to full height in one motion. Table 2.2 gives the different categories and world records of weight lifted in jerk and snatch motion for each of the seven categories. If there are enough lifters in each category, separate competitions can be run for each category. What contest is possible if there are too few competitors for separate competitions in each category? What is the greatest athletic achievement of a group of weight lifters of widely differing weight?

One solution to this problem would be a single competition for all weight categories with the winner decided using a handicapping rule designed to compensate for any body weight advantage. The problem is then to develop a meaningful handicap rule based on the data given in Table 2.2.

2.2 Case Study B (Alloy Selection)

Titanium alloy is used in the manufacture of high-precision components for many industries. Alpha Inc., a company specializing in metallurgical processes, has decided to set up a plant to produce titanium alloy. The alloy can be produced by two different methods and Alpha Inc. has the option of choosing the ore from four different mines. Alpha Inc. is interested in producing the alloy with the smallest thermal coefficient. The problem facing Alpha Inc. is to decide:

- (i) on the method to be used, and
- (ii) on the mine from which it must get the ore.

2.3 Case Study C (Optimal Production)

Milk can be consumed either directly or in processed forms such as cream, yoghurt and cheese. Beta Inc. is the sole producer of milk in a certain region and also owns the factory to process the milk into various forms. Beta Inc., like any other company, wants to maximize its total profit. The problem for the company is to determine the relative quantities of the various products necessary to achieve this goal.

2.4 Case Study D (Rocket Launch)

For meteorological purposes, rockets are launched so that they reach a certain altitude and record atmospheric conditions such as temperature and pressure. The problem here is to calculate the rocket thrust necessary to ensure that the rocket reaches the desired altitude.

2.5 Case Study E (World Population)

Many world organizations, for example the United Nations and its agencies, deal with global issues such as total food production and consumption of non-

TABLE 2.3 Data for Case Study E: Total World Population (1850–1980)

Year	Population (millions)
1850	1262
1900	1650
1920	1860
1930	2069
1940	2295
1950	2515
1960	2998
1970	3651
1980	4368

renewable resources. Growth in the world population is important in all such issues. Table 2.3 gives statistics for the world population for the last 100 years. The problem here is to obtain estimates for the total population for the next 100 years, with and without birth control policies.

2.6 Case Study F (River Pollution)

Gamma Inc. is a company which produces chemicals and is located on the banks of a river. In the past it has disposed of its waste by indiscriminately dumping it into the river, causing high levels of pollution. As a consequence, the local authorities passed new legislation with very high fines if the pollution in the river exceeded certain specified concentration limits. The problem here is to find a policy for discharging the waste so as to ensure that the concentration levels never exceed the specified limits.

2.7 Case Study G (Weather Changes)

The operators of a holiday resort complex have been using liquid fuel for heating their swimming pool so that the temperature of the pool is around 27 degrees Celsius. Due to the rising cost of liquid fuel, they have decided to look at alternative methods of heating the pool. Solar energy offers one such alternative. However, 8 hours of sunshine per day are needed for the pool to be maintained at the desired temperature. On days when the sun is shining for less than 8 hours liquid fuel must still be used to make up for the lack of solar heat. The operators have collected information regarding sunshine over an interval of 63 days. The information is as shown in Table 2.4, where each day is classified as being sunny (if there was 8 or more hours of sunshine); partly sunny (if the sunshine was between 4 and 8 hours) or cloudy (if the sunshine was for less than 4 hours). The problem of interest to the operators is to decide whether it is economical to install the solar heating system.

TABLE 2.4 Data for Case Study G: Weather Changes in the Holiday Resort

Week	Day						
	1	2	3	4	5	6	7
1	S	S	S	P	C	S	S
2	S	P	C	P	S	P	S
3	S	S	S	C	P	S	C
4	P	C	S	S	S	P	C
5	C	P	P	C	C	P	S
6	S	S	C	S	S	S	P
7	S	S	P	S	C	C	S
8	P	S	S	S	P	S	S
9	P	C	S	S	C	P	S

S: Sunny; P: partly sunny; C: cloudy.

2.8 Case Study H (Thermal Power Station)

A thermal power station is a large complex system which produces electricity by burning coal. Basically, the heat released by the burning coal is used to convert water into steam, which in turn drives a turbine to produce rotational motion. This motion causes a generator to convert the mechanical energy into electrical energy. Many problems arise in this context. A few are given below:

- For economic planning: when should the next power station be built, how large should it be and where should it be put?
- For control purposes: how does the alternator or boiler respond to fluctuating load?
- For design purposes: for a given output what is the necessary size of boiler and superheater?

2.9 Case Study I (Component Reliability)

Large complex machines, such as computers or rockets, are composed of a large number of components. Components are prone to failure, and the time to failure (or the age at failure) is uncertain and unpredictable. Table 2.5 gives the age at failure for a sequence of failures of a control element for a large machine. The machine is inoperable without this element. Thus, whenever the element

TABLE 2.5 Data for Case Study I: Age at Failure for Control Element ($\times 100$ hours)

1.8487	0.3761	0.7500	3.0530	1.3545
1.8802	1.5700	1.7708	1.3592	3.0466
1.7961	1.5319	0.5903	0.6288	0.6461
1.6560	1.7172	1.9310	1.0509	1.6173
1.3162	0.7705	1.8889	1.7410	4.1515

fails, it is replaced by a new one so that the machine becomes operable. The problem is to evaluate:

- how long the machine can be kept operational if there are n spares of the control element,
- how many replacement elements are needed to keep the machine operational for T units of time.

2.10 Case Study J (Speed of Aeroplanes)

In modern industrial society changes are taking place at a very rapid rate. One example of this is the increase in aircraft speed over the years. Table 2.6 gives the maximum speed of aircraft as a function of time from 1906 to 1965. Frequently military and civil aviation planners need to know what performance aircraft are likely to have at some future time, say in the year 2000. The problem here is to predict the likely maximum speed in the year 2000.

2.11 Case Study K (Supermarket Operation)

In large supermarkets there are usually a large number of normal, and a few fast, checkout counters. People with less than a specified number of items stand in line at fast checkout counters, while others go to normal checkout counters. Fewer counters imply long queue lengths and this can affect customer goodwill. On the other hand, if there are too many checkout counters, manning them reduces the total profit. The problem is to decide on the optimum number of checkout counters that the supermarket should have.

2.12 Case Study L (Demand for Soft Drinks)

Cool Inc. is a company which manufactures soft drinks. It is thinking of expanding its plant capacity so as to meet future demands. The monthly sales for the past 5 years are given in Table 2.7. The problem is to obtain good estimates for future demand so as to help the company make the right decision.

3 Need for a Unified Approach

As seen from the case studies of the previous section, each problem is distinct and differs from any other. A comprehensive framework, to treat such distinctly different problems in a unified manner, is highly desirable and indeed essential. The systems approach offers such a framework.

In the systems approach, the real world associated with the problem is viewed as a system. Identifying the features of the system that are relevant for the problem is called system characterization, and is discussed in the next chapter.

TABLE 2.6 Data for Case Study J: Speed of Aeroplanes

Date	Country	Speed (mph)
Nov. 12, 1906	France	25.66
Oct. 26, 1907	France	32.75
May 20, 1909	France	34.06
Aug. 23, 1909	France	43.38
Aug. 24, 1909	France	46.18
Aug. 28, 1909	France	47.84
Apr. 23, 1910	France	48.21
July 10, 1910	France	66.18
Oct. 29, 1910	United States	68.20
Apr. 12, 1911	France	69.47
May 11, 1911	France	74.42
June 12, 1911	France	77.67
June 16, 1911	France	80.91
June 21, 1911	France	82.73
Jan. 13, 1912	France	90.20
Feb. 22, 1912	France	100.22
Feb. 29, 1912	France	100.94
Mar. 1, 1912	France	103.66
Mar. 2, 1912	France	104.33
July 13, 1912	France	106.12
Sept. 9, 1912	United States	108.18
June 17, 1913	France	111.73
Sept. 27, 1913	France	119.24
Sept. 29, 1913	France	126.67
Feb. 7, 1920	France	171.04
Feb. 28, 1920	France	176.14
Oct. 9, 1920	France	181.86
Oct. 10, 1920	France	184.36
Oct. 20, 1920	France	187.98
Nov. 4, 1920	France	192.01
Dec. 12, 1920	France	194.52
Sept. 26, 1921	France	205.22
Sept. 21, 1922	France	211.90
Oct. 13, 1922	United States	222.97
Feb. 15, 1923	France	233.01
Mar. 29, 1923	United States	236.59
Nov. 2, 1923	United States	259.15
Nov. 4, 1923	France	266.58
Dec. 11, 1924	France	278.48
Sept. 5, 1932	United States	294.38
Sept. 4, 1933	United States	304.98
Dec. 25, 1934	France	314.319
Sept. 13, 1935	United States	352.388
Nov. 11, 1937	Germany	379.626
Mar. 30, 1939	Germany	463.917
Apr. 26, 1939	Germany	469.220
Nov. 7, 1945	Great Britain	606.255
Sept. 7, 1946	Great Britain	615.778
June 19, 1947	United States	623.738
Aug. 20, 1947	United States	640.663
Aug. 25, 1947	United States	650.796
Sept. 15, 1948	United States	670.981
Nov. 19, 1952	United States	698.505
July 16, 1953	United States	715.745

TABLE 2.6 (Contd.)

Date	Country	Speed (mph)
Sept. 7, 1953	Great Britain	727.624
Sept. 25, 1953	Great Britain	735.702
Oct. 3, 1953	United States	752.943
Oct. 29, 1953	United States	755.149
Aug. 20, 1955	United States	822.266
Mar. 10, 1956	Great Britain	1132.136
Dec. 12, 1957	United States	1207.6
May 16, 1958	United States	1404.09
Oct. 31, 1959	U.S.S.R.	1483.85
Dec. 15, 1959	United States	1525.965
Nov. 22, 1961	United States	1606.48
July 7, 1962	U.S.S.R.	1665.9
May 1, 1965	United States	2070.102

TABLE 2.7 Data for Case Study L: Monthly Sales ($\times 1000$ litres)

Month	Year				
	1983	1984	1985	1986	1987
January	629	747	874	997	1095
February	642	781	896	1008	1102
March	693	812	936	1044	1146
April	694	811	952	1054	1154
May	682	822	932	1043	1138
June	686	814	929	1040	1142
July	689	815	938	1062	1139
August	718	826	940	1048	1172
September	743	852	944	1076	1168
October	755	878	999	1092	1148
November	767	852	994	1082	1170
December	739	805	986	1124	1192

Notes and References

The problems discussed in this chapter, though varied, do not cover all disciplines of learning. For example, literature, law, and health are a few not represented. A problem in literature where mathematics and computing has proved to be extremely useful is the following. Is an old text (e.g. a book of the Old Testament) written solely by a single author, or is it the work of multiple authors? Mathematical models can be built to answer such questions. Interested readers can find details of such models in [1] and [2].

Problems can be classified in two ways. Firstly, they can be classified by the discipline to which they belong – for example, social science, biological science, technology and so on. Further subdivisions exist – for example, in the

case of technology it would be chemical engineering, mechanical engineering, civil engineering and so on. Secondly, problems can be classified into different groups based on the nature of the problem – for example, problem of analysis, of synthesis, of optimization, of forecasting, to name a few.

For additional problem definitions see Chapter 17.

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CHAPTER 3

System Characterization

1 Introduction

In the previous chapter we described a large number of real-world problems in the form of Case Studies A–L, and mentioned that the systems approach offered a universal framework for treating such distinctly different problems. In the systems approach the real world associated with the problem is viewed as a system, and the solution to the problem as a study of the system with a defined goal. The starting point for such a study is a proper description of the system.

In order to describe the system, one needs a clear understanding of the terms and concepts used in the systems approach and the precise meaning attached to them. Also, any significant problem in its real-world form is usually very complex. Hence, a total description of it, when viewed as a system, becomes involved and unmanageable. Fortunately, not all features of the real world are relevant to the problem or its solution. Consequently, a partial description is often adequate. This partial description, called the “system characterization”, retains only those features of the real world that are relevant for the problem to be solved. Thus, the system characterization phase, as shown schematically in Figure 3.1, can be viewed as a process of simplification, and idealization.

The system characterization can be done in any natural language, for example English. However, alternative methods, such as schematic or graph-theoretic or matrix representation, are more compact and elegant representations. As such they present the problem in a form that is easier to comprehend and facilitate the first conceptual steps towards mathematical model building.

In this chapter we describe the process of system characterization. We discuss various terms and concepts used in the systems approach and make the meaning clear by applying them to Case Studies A–L introduced in the previous chapter in the form of examples.

2 Some Basic Concepts

In this section we start by defining a system, and discuss some basic terms and concepts used in the systems approach. In subsequent sections we discuss

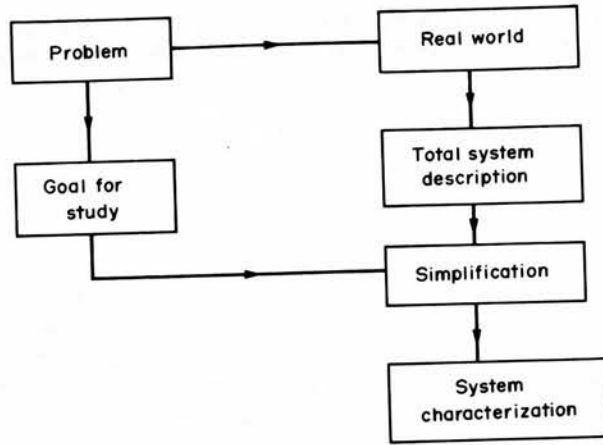


FIGURE 3.1 Systems approach to real-world problem solving.

further concepts that play an important role in developing a system characterization.

2.1 System/Variable/Parameter

A “system” can be defined as a collection of one or more related objects. An object is a physical entity with specific characteristics or attributes. The objects can be either non-interacting or interacting in some sense. Of special interest are systems where there is interaction between the objects, since these most closely resemble the real world.

The attributes of an object are described in terms of “parameters” and “variables”. Parameters are attributes intrinsic to an object. Variables are attributes needed to describe interaction between objects. Often, parameters and variables are terms from some theory or theories, if such exist, and are used to explain the state and behaviour of the system. When no such theory exists, variables and parameters are words from a natural language with the usual meaning. We will illustrate these points by a few examples.

Example 1 (Thermal Power Station: Case Study H)

A thermal power station can be viewed as a system which, in functional terms, may be reduced to three main objects – boiler, turbine and generator. The variables and parameters to describe the attributes of the first two objects are terms from the theories of heat transfer, fluid mechanics and dynamics, while for the last object they are terms from the theories of dynamics, electricity and magnetism.

Example 2 (Supermarket Operation: Case Study K)

A supermarket, viewed as a system, is a collection of basically three different types of objects – customers, checkout counters and products for sale. The variables are the number of customers in

the shop, number of customers waiting at the counters, number of items purchased by each customer and so on. Two system parameters are (i) the price of each product and (ii) the number of counters.

Example 3 (Component Reliability: Case Study I)

The control element can be viewed as a single-object system. The variables describing the system would be the state of the element – i.e. working or failed, and the age of the element if it is working.

2.2 System/Environment

The way we have characterized a “system”, so far, implies that it is either an isolated single object or an isolated collection of objects. In reality this is seldom the case. The system under study is usually a subset of some bigger system – more appropriately labelled a “super-system”. This super-system is usually the observer and the universe known to him or her.

The objects in the system under study might or might not interact with objects of the super-system which do not belong to the system. The system is said to be a “closed system” if there is no such interaction and an “open system” if there is.

The “system environment” is the term used to describe those objects that are outside the system but interact with it. The interaction between the system and its environment is through variables common to both. This raises the natural question – When does an object belong to the system and when does it belong to its environment? If an object interacts with the system in the way described above, should it not be considered a part of the system, since the system and its environment make up the universe of interest. Subdivision of this into two parts – system and environment – is mainly for convenience and quite arbitrary, since the division can be done in many ways. We will illustrate this by a few examples.

Example 4 (Thermal Power Station: Case Study H)

The thermal power station produces electricity from coal. The coal is obtained from mines. The generated electricity is fed into a distribution network which distributes the electricity to users. We can regard the coal mine as an object outside the system which affects the system. The network is regarded as another such object but, in this case, is affected by the system. The system becomes more complicated if we include these objects within its boundaries.

Often diagrammatic displays are more effective than natural language in describing the system.

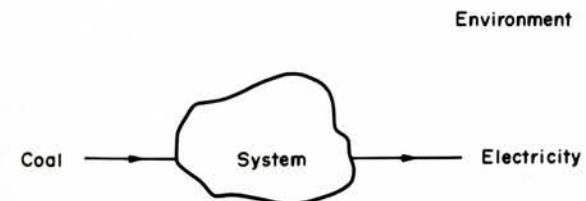


FIGURE 3.2 System/environment interface for Example 4.

One such display is shown in Figure 3.2, where the separation between the system and its environment is shown by a closed curve. The interactions between the system and its environment are shown by directed arrows. The direction of the arrow shows the type of interaction – system affecting the environment or vice-versa. (We shall discuss interaction in a later subsection.)

The reason for this division is that, in our study of a power station system, we do not care how the coal is mined and delivered or how the electricity is used. Hence these are treated as belonging to the environment.

Example 5 (Weight Lifting: Case Study A)

The real world of the problem can be viewed as a system with two objects – i.e. the weight lifter and the weights for lifting. The variables describing the attributes of the objects are the body weight of the lifter and the weight lifted. Since the interest is on weight lifted, we can view the system as a closed one, for no objects outside the system are of importance.

Note that the object "weight lifter" has many other attributes, for example height, colour of his skin etc.; but these are of no importance and can be ignored. This illustrates the process of simplification mentioned in Section 3.1.

Example 6 (Demand for Soft Drinks: Case Study L)

When the real-world problem in this case study is viewed as a system, one variable of importance is the periodic (weekly, monthly or yearly) demand for the product. If future demands are characterized solely in terms of past sales, then we view the system as a closed system. On the other hand, if one includes variables such as population changes, weather conditions, advertising etc., then we view the system as an open one, as shown in Figure 3.3.

These examples show particular choices of system boundary which are satisfactory for the problems in question. Other boundaries could have been chosen but would have led to different characterizations. The selection of a system boundary is one component of the art aspect of mathematical modelling – there is no universally correct division between system and environment. Novel and useful characterizations can follow from different choices of system boundary.

2.3 Relationships (Interaction between Objects)

The interactions between objects are described through relationships linking the variables of the interacting objects. Of particular importance are "cause-

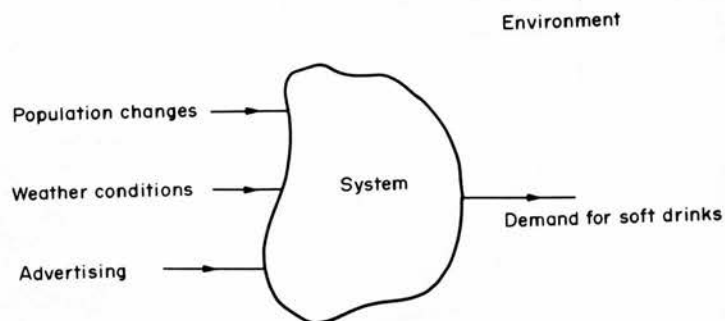


FIGURE 3.3 System/environment interface for Example 6.

effect" interactions producing what are termed "causal relationships". Such a relationship may be illustrated by the following well-known proverb:

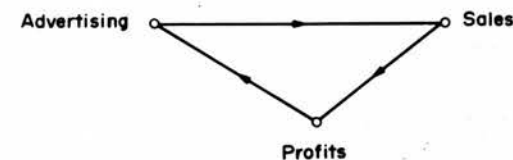
For want of a nail a shoe was lost; for want of a shoe a horse was lost; for want of a horse a rider was lost; for want of a rider a battalion was lost; for want of a battalion a battle was lost; for want of a victory a kingdom was lost – all for want of a nail.

Causal relationships are best indicated by means of either graph-theoretic or matrix tabular displays, as shown by the following examples.

Example 7 (Advertising)

Companies use advertising to improve their sales, and hence revenue and profits. However, advertising is an expensive operation affecting company profit. The problem in advertising is to decide how much and what kind of advertising is justified. From the systems approach point of view the real world of the advertising problem can be viewed as a closed system with three variables – sales, profits and advertising expenditure. Advertising expenditure affects sales, which in turn affects profits. The profits, in turn, affect advertising expenditure. We can display the causal relationships, very elegantly and compactly, by using a graph-theoretic display, as shown in Figure 3.4. In this display nodes represent variables, and directed arcs indicate the causal relationships. The direction of the arrow points away from the variable which is the cause and towards the variable which is being influenced. We will find that graph-theoretic representations of this kind are extremely useful in succinctly characterizing the system under study.

Graph-theoretic display



Matrix tabular display

	Advertising	Sales	Profits
Advertising	0	1	0
Sales	0	0	1
Profits	1	0	0

FIGURE 3.4 Alternative displays for Example 7.

An alternative representation of the advertising problem is a matrix tabular display, also shown in Figure 3.4. Here, an entry "one" corresponds to a causal relationship, with the row variable being the cause and the column variable being the one getting affected. An entry "zero" corresponds to no such causal relationship.

In some systems (especially those associated with problems in social sciences) it is not easy to identify and define causal relationships between variables. In some cases there can be more than one cause for an effect, as illustrated by the following example.

Example 8 (Death of Pedestrian)

Suppose a car has struck a pedestrian in a darkened street of a city, resulting in his death. What was the cause of the death for the pedestrian? One answer would be that the pedestrian was struck by a car. But if one asks – Why did the car strike the pedestrian? – we arrive at multiple cause-effect interactions. For example, a lawyer might say that it was negligence on the part of the driver; a car builder might say that it was due to a defective brake shoe which prevented the car from stopping in time; a city planner might say that it was due to a poorly designed road, whereas a doctor might say that it was due to alcohol. Which cause or causes are important depends on the goal or purpose of study.

3 Degree of Detail

Consider an open system that is described only by the variables through which it interacts with its environment, and the inner structure of the system is ignored. This description is called a "black-box" description. Such a situation occurs when one has very little understanding of the inner structure of the system. Even when there is some knowledge of the inner structure, it is still sometimes convenient to view it as a "black box" for the purpose of deriving a simpler description of the system. In either case the inner details are being ignored. On the other hand, if one can describe all the objects in the system and their attributes (through variables and relationships) then one is describing the system in greater detail. In this case the system is being viewed as a "white box" (in contrast to a "black box"). More appropriately, it should be called a "transparent box".

The degree of detail needed to describe a system appropriately depends on many factors. If all the details are included in the description it can become unmanageable and hence of limited use. However, if significant details are omitted the description is incomplete and, once again, of limited use in carrying out the study. Hence, one needs to find a sensible compromise. The search for this compromise is a part of the "art aspect" of the modelling process. We illustrate these points by a few examples.

Example 9 (Component Reliability: Case Study I)

For this problem we have two different system characterizations based on the degree of detail included. The first is a simple characterization with only one variable – the state of the element, which can assume only two values – one or zero. Zero corresponds to a failed state and one to a working state. In the second we describe the mechanism of failure, e.g. crack propagation, if the

failure is due to a crack in metal. This would result in a more detailed description with more variables and relationships.

Example 10 (World Population: Case Study E)

For this problem a system characterization which differentiates the population by (i) age, (ii) sex and (iii) geographic location contains more details of the real world than a description where all these are lumped together.

4 Static vs Dynamic

In static systems time does not play any part, and hence the variables and relationships describing the system are time-independent. In contrast, in dynamic systems, time plays a very important role with the variables and/or relationships describing the system changing with time. We illustrate by considering two examples.

Example 11 (Alloy Selection: Case Study B)

The problem can be described in terms of a closed system with three variables.

- A: coefficient of expansion for the alloy,
- B: method of production,
- C: supplier.

The causal relationships between the variables are as shown in Figure 3.5. In this description time plays no role and hence the system is a static system.

Example 12 (Rocket Launch: Case Study D)

The problem can be described in terms of a closed system consisting of two objects – the rocket and the earth. The variables describing the rocket are its position and velocity relative to some fixed point on the earth, and the interaction between the two objects is given by the theory of dynamics. In this description we have excluded the influence of other planets in the solar system. If these influences are important we can include them by treating the planets as belonging to the environment of the system and the system being viewed as an open system (as opposed to a closed system). In either case the variables – i.e. position and velocity of the rocket – change continuously with time. Hence the system is a dynamic system.

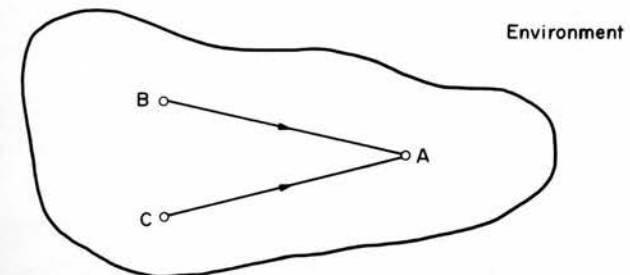


FIGURE 3.5 Graph-theoretic display of causal relationship for Example 11.

In dynamic systems time enters into the cause-effect interactions. Let x and y represent two variables of a dynamic system with changes in x over time being the cause for changes in y over time. Since only the past can influence the present and the future, and not the reverse, $y(t)$ (the variable y at time t) is affected only by $x(\tau)$ with $\tau \leq t$ and not by $x(\tau)$ with $\tau > t$. This is called the "principle of causality", which all physical systems obey.

4.1 Continuous Time vs Discrete Time

In dynamic systems either some or all of the variables are changing with time. One may ask whether the changes take place continuously with time or whether they occur at discrete instants of time. Experimentally, it is not possible to establish that a variable is changing continuously with time, since we are restricted by some finite resolution of time for each observation. Thus, one has to make an *a priori* decision whether to treat the time element as continuous or discrete. If the time element is treated as being continuous, then the variables of the system need to be described for all time instants over the time interval of interest. On the other hand if it is treated as being discrete, then the variables need to be described only for the relevant time instants.

A continuous time description is too detailed in many instances. In such situations one chooses a discrete time description by arbitrarily discretizing the time. If the interval of discretization is large one obtains a coarse description. As this interval becomes smaller the description becomes more refined and detailed, and ultimately approaches the continuous time description.

The decision to treat the time element as continuous or discrete is often a subjective one, and once again involves the art aspect of modelling. However, in certain instances the data available are such that a discrete treatment of time is the most appropriate decision. We illustrate this point by a few examples.

Example 13 (Demand for Soft Drinks: Case Study L)

If one is interested in weekly demand, then the variables of the system characterization change weekly, and hence the time element is to be treated as discrete as opposed to continuous. Obviously, if the demand interval is monthly, then the interval of discretization is larger, resulting in an aggregate or coarser description.

Example 14 (River Pollution: Case Study E)

The river pollution problem is best described by treating the time element as being continuous with the variables of the system description (e.g. concentration level in the river at a given location) changing continuously with time.

4.2 Time Scales in Dynamic Systems

In dynamic systems the variables change with time. The term "time scale" is used to indicate the duration for significant changes to occur in a variable.

TABLE 3.1 Time Scales for Example 16

Time scale of interest	Relevant theory for interaction
$\tau_0 = r_0/u$ (Collision time scale)	Particle dynamics (Deterministic and reversible)
$\tau = \lambda/u$ (Kinetic time scale)	Kinetic theory (Statistical and reversible)
$T = L/u$ (Macroscopic time scale)	Continuum theory (Field theory and phenomenological)

Often, when variables change at different rates, there can be more than one time scale.

If the time interval of study is T , then variables with time scales very much larger than T can be approximated as not changing over the time interval of study, thus reducing the number of dynamic variables needed in the characterization. Variables with time scales smaller than T , or comparable to T , need to be described for all time instants as they change significantly over the time interval of study. Identifying the different time scales is a part of system characterization.

Example 15 (Thermal Power Station: Case Study H)

Suppose that the problem is to design an efficient boiler. In the systems approach the boiler can be viewed as a system consisting of many objects – coal particles, burner, heat exchange tubes, boiler drum, etc. Typically the heat is released by the burning of coal particles in a coal-fired power station. The typical size of coal particles is $\sim 50 \mu\text{m}$. The process of heat release is complex. First, the particle goes through a process of volatilization, during which hydrocarbon gases are released and the coal is transformed into char. Depending on particle size, the time scale (T_1) for this is typically ~ 20 ms. Then the char burns to ash and typically the time scale (T_2) for this is ~ 200 ms. Since the coal particles and ash are transported in a stream of hot gases, we have a third time scale (T_3) – the duration for which the particle (initially as coal, then as char and finally ash) stays in the boiler. This duration is given by the length of path that the particle has to traverse in the boiler divided by the mean velocity of the hot gases. Proper design requires that $T_3 > T_2 + T_1$, or else heat is wasted in the chimney.

Example 16 (Magnetohydrodynamic System)

The operation of a magnetohydrodynamic (MHD) system can be described by the motion of charged particles (ions and electrons) orbiting the lines of a magnetic field. There are at least five different length scales, such as the range of interparticle potential r_0 ; the mean free path λ ; the two radii of gyration $r_{Le} = u_e (eB/M_e)$ and $r_{Li} = u_i (eB/M_i)$ where $u_e [u_i]$ and $M_e [M_i]$ are the mean thermal speed and mass of electron [ion] and the macroscopic length L (the size of the system); e is the charge of electron and B is the strength of magnetic field. On dividing these lengths by u_e and u_i we arrive at a set of time scales. Thus for the electron (and similarly for the ion) we have the hierarchy of time scales as shown in Table 3.1. The two other gyro-times M_e/eB and M_i/eB can lie anywhere on the time scales. Table 3.1 also shows the relevant theories needed to describe the interactions in the system.

5 Deterministic vs Stochastic

A system is said to be deterministic if the values assumed by the variables (for a static system) or the changes to the variable (for a dynamic system) are

predictable with certainty. If not, then uncertainty is a significant feature of the system and the values assumed by the variables, or the changes in the variable, are random and unpredictable. Such systems are called either probabilistic or stochastic systems.

In real life there is always uncertainty. If the uncertainty is insignificant then it can be ignored and the system can be treated as a deterministic system. This is a process of simplification or idealization. If the uncertainty is significant then it cannot be ignored and must be taken into account in the system characterization.

Example 17 (Component Reliability: Case Study I)

As discussed earlier, the component can be viewed as a single-object system with the time to failure as one of the variables describing the system. The data in Table 2.5 indicate that there is a large variability in the time to failure; hence the system must be viewed as a stochastic system.

Example 18 (Rocket Launch: Case Study D)

The variables of the system are the position and velocity of the rocket. Since the laws of classical dynamics describe the motion fairly accurately, the changes in position and velocity can be predicted with a high degree of certainty. Hence, in this case we can view the system as being deterministic.

6 System Characterization of Case Studies A–L*

In this section we carry out the system characterization of the real-world problems defined in Case Studies A–L in Section 2 of Chapter 2. These system characterizations will be used later in Chapters 5 and 7 to build mathematical models.

6.1 Case Study A [Cont.] (Weight Lifting)

The weight (L) lifted by a weight lifter in either jerk or snatch motion depends to a large extent on his body weight (W) and to a small extent on various other factors – some internal to the weight lifter and others external. Some of the internal factors are the physical and mental conditions of the lifter, while some of the external ones are the physical conditions of the location where the competition is taking place and the spectator response. Often these external factors play a very minor role and hence can be ignored. As a consequence the problem can be described in terms of a closed system with two objects – the weight lifter and the weight.

Since the interest is in the weight lifted in jerk and snatch motions, the time history of the motion is of no significance; hence the system can be viewed as a static system. Also, since a weight lifter can repeat his best lifts with a fair degree of predictability, we can treat the system as a deterministic system.

*See footnote on page 10.

The simplest description involves only two variables – the body weight of the lifter (W) and the weight lifted (L). The weight lifted is different for snatch and jerk motions as in the snatch the weight is pulled from the floor to a locked overhead position in a single move; whereas for the jerk two moves are allowed – the first to the chest and the second to the overhead position. A slightly more detailed description is one where the body weight is divided into two components – muscular and non-muscular.

The goal for the study is to find a handicapping rule to decide the winner when body weights of competitors vary significantly. We do this by finding a relationship between L and W using the data given in Table 2.2 and then obtaining the handicapped weight lifted (L') by scaling L in terms of W using the relationship. The winner can then be decided on the basis of the highest score for L' .

6.2 Case Study B [Cont.] (Alloy Selection)

Alpha Inc. is interested in producing titanium alloy with the least possible thermal coefficient. As there is more than one method of producing titanium alloy and more than one source for the ore needed, the problem facing Alpha Inc. is first to establish whether there are significant differences in the thermal coefficient of alloys produced by different combinations of ore and method of production. If the differences are not significant the decision is simple, since it does not matter from which mine the ore is obtained or the method of manufacture. When the differences are significant, the decision is again simple if, for each combination of ore and method, the variability in the thermal coefficient is small and insignificant. In this case the particular combination of ore and method which yields the smallest value for the thermal coefficient is the one that Alpha Inc. should select.

We will consider here the more complicated case in which the thermal coefficient varies significantly for all combinations of ore and method of manufacture. This could be due to many factors – the variability in the ore due to geological conditions and variability in the method of manufacture due to uncontrollable factors. These variations are unpredictable; hence the variations in the thermal coefficient of the alloys are also unpredictable.

In this case the problem can be described in terms of a closed system with four significant variables: (i) the mine from which the ore is obtained (MA), (ii) the method used in manufacture (ME), (iii) the thermal coefficient of the alloy (TC) and unknown influences (X). Other variables can be ignored as Alpha Inc. has no control over them and their effect on TC is accounted for through X .

The four different mines can be labelled as MA_i ($i = 1, 4$) and the two methods as ME_j ($j = 1, 2$). As a result we have eight different alloys – obtained by different combinations of manufacturer and method. These we label as TC_{ij} ($i = 1, 4; j = 1, 2$) with TC_{ij} representing the thermal coefficient of the alloy

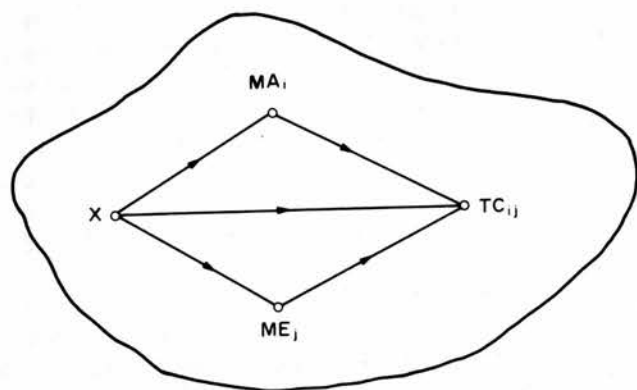


FIGURE 3.6 System characterization for Case Study B.

produced by using ore from MA_i and method ME_j . TC_{ij} is a random variable due to the influence of X .

Following the standard terminology of the design of experiment, we shall call "ore from mine" and "method" factors which affect the thermal coefficient of the alloy.

Since Alpha Inc. is interested only in the thermal coefficient of the alloy, time plays no role; hence the system can be viewed as a static system. The relationship between the variables is as shown in Figure 3.6, indicating that the method and the manufacturer can affect the thermal coefficient of the alloy.

The goal of the study is first to establish whether ore from different mines and method of manufacture affect the thermal coefficient significantly; and second to determine the right decision that Alpha Inc. must make with regard to the ore and the method of manufacture.

6.3 Case Study C [Cont.] (Optimal Production)

Beta Inc. manufactures a range of products from milk. Since the aim of Beta Inc. is to maximize profits by varying product distribution, an important variable is the time interval over which the company wishes to maximize its profits. Let T denote this time interval. If T is sufficiently large, then it can be approximated as being infinite, and the aim is then to maximize the profits per unit time. The reason for treating the time interval as being infinite is that this allows the use of asymptotic methods to obtain the optimal solution. If T is not sufficiently large, then this approximation is not valid. In either case the variables of the system characterization, when the real world associated with the problem is viewed as a system, change with time. Thus, time is an important element and the system must be treated as a dynamic system.

The time element can be treated as either discrete or continuous. Continuous time characterization is too detailed and hence not appropriate. The unit of discretization could be either a day, week or month. There could be

significant day-to-day variations in the delivery of certain products, payments received and so on. The delivery variations are made possible by shelf-life of many days for most products. Clearly a day unit would provide a more detailed description than is necessary for profit optimization. Most of these fluctuations, irrelevant to the present study, would disappear if a week was chosen as the unit of discretization. A month would be too long and information about the factory performance would be lost with such a coarse unit of discretization. For these reasons a week is the most appropriate time interval of discretization for the problem.

If we assume that there is no carry-over from week to week, then each week can be treated independently. Hence the aim of maximizing profits over the interval T is equivalent to maximizing profit for each week separately. As a result we can ignore the dynamic nature of the system and treat the operation over each week using a static characterization, thus making the system characterization a lot simpler.

We use the following notation to represent aggregate weekly values.

- X : milk delivered to factory (in litres)
- Y_1 : milk used for producing butter (in litres)
- Z_1 : amount of butter produced (in kilograms)
- S_1 : amount of butter sold (in kilograms)
- D_1 : demand for butter (in kilograms).

Similarly, Y_2 , Z_2 , S_2 and D_2 correspond to yoghurt; Y_3 , Z_3 , S_3 and D_3 correspond to cream.

- Y_4 : milk used for sale as processed milk (in litres)
- D_4 : demand for processed milk (in litres).

The system characterization for the problem is as shown in Figure 3.7. Note that the system is an open one with five input variables (X and D_i , $i = 1, 4$) and four output variables (S_i , $i = 1, 4$). The remaining variables are internal to the system. The parameters of the system are c_p , s_j and T_j ($j = 1, 3$) with c_1 representing the cost of producing one unit of butter; s_1 representing the selling price of one unit of butter; T_1 representing the number of units of milk required to produce one unit of butter and so on. c_0 represents the cost of producing one unit of milk before processing.

In the system characterization shown in Figure 3.8a for the case of butter production we have the sale price for the products fixed and not affected by the amount produced. However, the amount sold is affected by the sale price. Since it makes no sense to produce more than the demand, as there is no carry-over from week to week, we have constraints of the form $Z_i \leq D_i$ ($i = 1, 4$). In addition we have various other constraints – e.g. $Y_1 + Y_2 + Y_3 + Y_4 < X$ and so on.

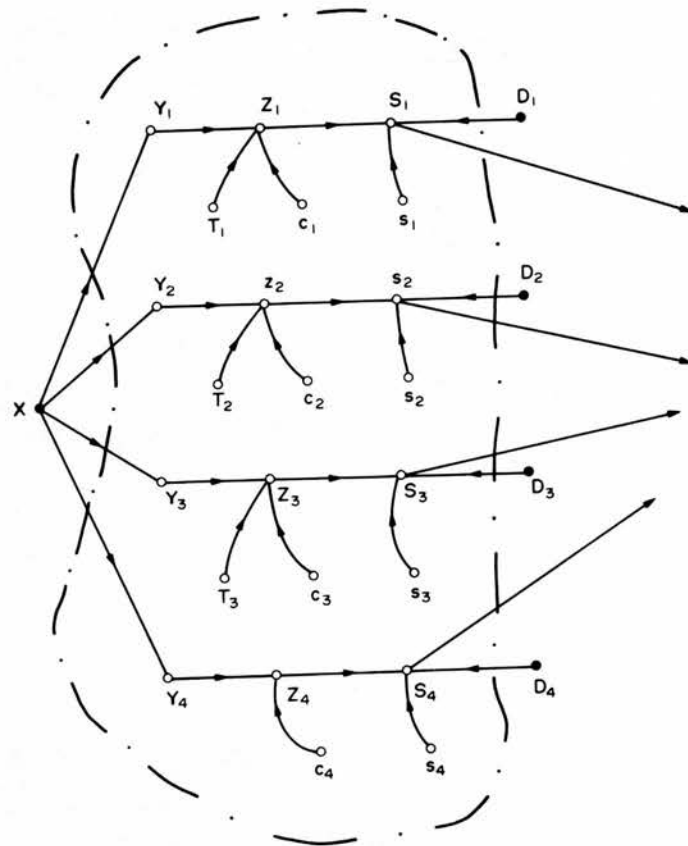


FIGURE 3.7 System characterization for Case Study C.

On the other hand, if the sale price is influenced by the quantity produced, then prices need to be treated as variables with a causal relationship, as shown in Figure 3.8b. Similar relationships hold for other processed products.

If we assume that everything produced is sold, and that the uncertainty in demand is small, then we can treat the system as deterministic. In this case the problem is described in terms of an open deterministic static system.

The goal for the study is to obtain the optimal $Y_i (i = 1, 4)$, for a given X , so as to maximize the profit which is given by the difference between the revenue generated by sales and the costs incurred.

Comment. If carry-over of products from one week to another is allowed, then we cannot treat each week separately. In this case the variables are sequences, i.e. $Z_1(i)$, $i = 1, 2, \dots$ represents the amount of butter produced in week i . Because of carry-over we need a set of additional variables representing the level of stocks of different processed products at the end of each week.

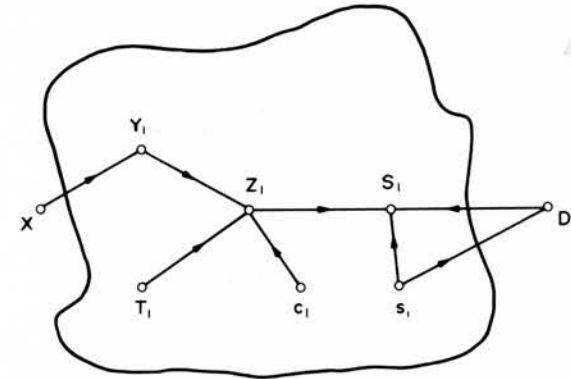


FIGURE 3.8a Partial system characterization for Case Study C (selling price fixed).

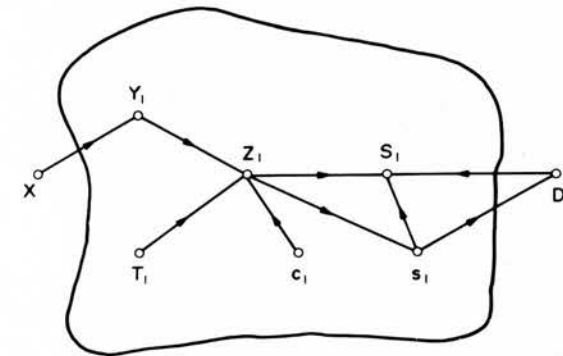


FIGURE 3.8b Partial system characterization for Case Study C (selling price not fixed).

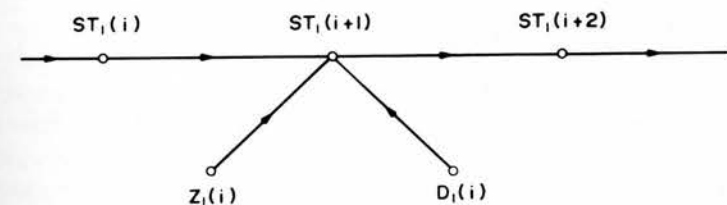


FIGURE 3.9 Partial system characterization for Case Study C (carry-over from week to week).

Thus, for the case of butter we would have an additional variable $ST_1(i)$ to represent the stock at the end of week i . The relationship between the variables associated with butter are as shown in Figure 3.9. In this case the system characterization is more complex than the one discussed earlier.

6.4 Case Study D [Cont.] (Rocket Launch)

The motion of the rocket is influenced by the thrust generated by it and the forces acting on it due to its interaction with the earth and other celestial bodies.

To start, let us assume that the forces due to interaction with celestial bodies (other than the earth) are insignificant. This is a process of simplification, and the validity of this assumption needs to be established at a later stage. With this assumption a description of the problem can be done in terms of a closed system with two objects, the rocket and the earth, each interacting with the other. The variables characterizing the rocket are its position and velocity with respect to some fixed point on the earth and the thrust generated by the rocket. We can regard the point from where the rocket is launched as the fixed point. If we assume that the rocket is launched to move in a vertical direction, the position of the rocket is described by a single variable which changes with time as the rocket moves. Let $x(t)$ denote the altitude of the rocket at time t with $t = 0$ corresponding to the instant at which the rocket is launched. The velocity is given by $x'(t)$ – the time derivative of $x(t)$. Let $F(t)$ represent the thrust generated by the rocket in its upward motion.

Since the motion of the rocket is governed by the laws of dynamics, the acceleration of the rocket $x''(t)$, the time derivative of $x'(t)$, is influenced by the following three forces.

- (i) $F(t)$: thrust generated by the rocket,
- (ii) G : gravitational force of attraction,
- (iii) f : frictional retarding force.

The direction in which these forces act can differ depending on whether the rocket is going up or down, as shown in Figure 3.10.

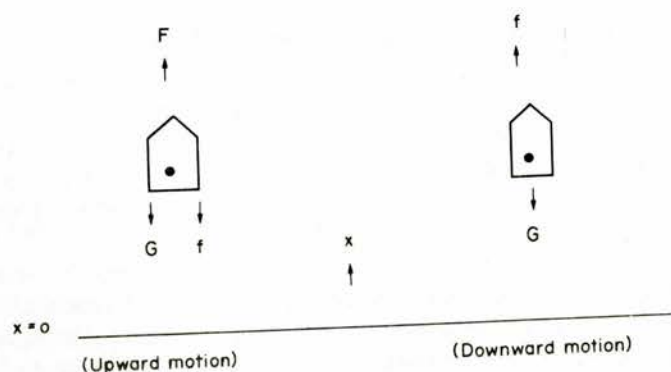


FIGURE 3.10 System characterization for Case Study D.

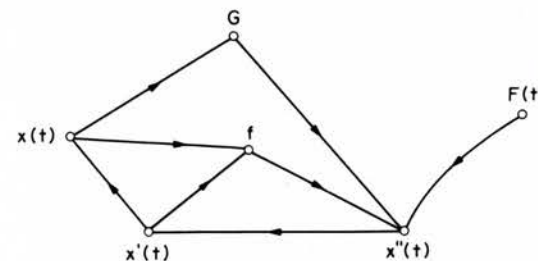


FIGURE 3.11 System characterization for Case Study D.

As a result the system characterization involves four variables. The relationship between the variables is given by the laws of dynamics. The gravitational force varies with x , whereas the retarding force depends on both x and x' . The relationship is as shown in Figure 3.11. The parameters of the system are the mass of the rocket and the constants of the functions which relate G to x and f to x and x' .

Note that if the forces due to interaction with other celestial bodies are significant, contrary to our assumption here, they can be included as additional variables acting on the system from the outside environment. In this case the system is no longer closed but is an open one.

In general, the thrust $F(t)$ is of constant magnitude F_m and acting for a relatively short period in relation to the time taken to reach the maximum altitude. In this case we can approximate the thrust as an impulse.

Since the position changes continuously with time, the time variable is best treated as being continuous. As the motion is predictable, the problem can be described in terms of a closed, dynamic and deterministic system. The goal of the study is to obtain the relationship between F_m and x_m – the maximum altitude reached. From this, one can calculate the thrust needed to ensure that the rocket reaches the desired altitude.

6.5 Case Study E [Cont.] (World Population)

The human population is continuously changing with time, increasing with each birth and decreasing with each death. With time, people age, and as a consequence the age structure of the population changes. In describing population changes one can treat the time variable as either continuous or discrete. We shall first deal with the case where time is treated as a continuous variable.

The simplest characterization is in terms of a closed dynamic system with human beings as objects, and characterized by one single variable, $N(t)$, the total population at time t , and two parameters – birth rate b and death rate d . The rate of change of population, $N'(t)$, is predictable and affected by $N(t)$, b and d as shown in Figure 3.12.

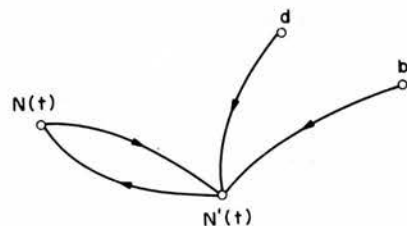


FIGURE 3.12 System characterization for Case Study E.

The above characterization is obviously not adequate to predict the population in 100 years time, since it ignores many relevant features of population change. One such is the constraint that the earth can support only a finite number of people. This can be included in the system characterization by including a new parameter, L , the upper limit to the population. As $N(t)$ reaches the level L the rate of change in population goes to zero.

A slightly more detailed characterization is one where the population is divided into different groups, based on sex. In this case we have two variables, $N_m(t)$ and $N_f(t)$, representing the total male and female numbers at time t . The two groups can have different birth and death rates.

A more refined characterization is one where the grouping is based on age instead of sex. The age structure can be characterized in two different ways. In the first and simpler characterization, we have three groups.

- group 1: young and juveniles
- group 2: mature and child-bearing
- group 3: old.

In this case the system is characterized by three variables – $N_i(t)$ ($i = 1, 3$) with $N_i(t)$ representing the number of people in group i at time t . The system

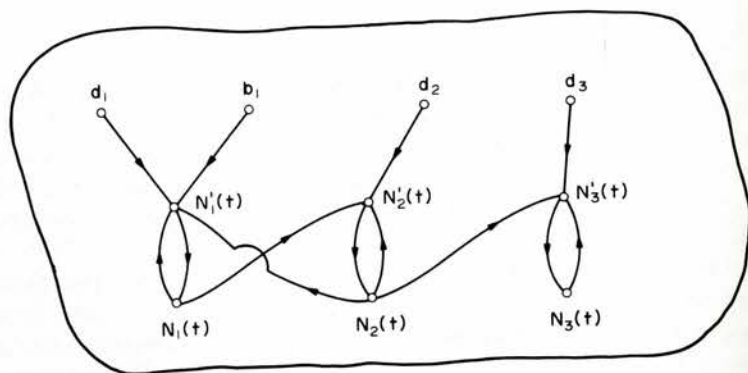
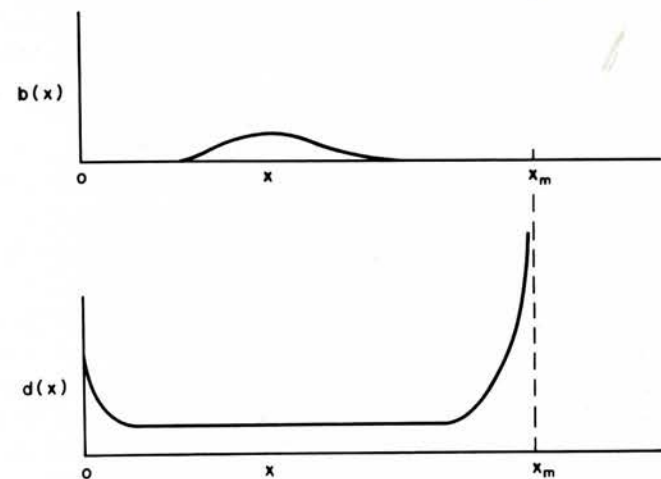


FIGURE 3.13 System characterization for Case Study E (age structure included).

FIGURE 3.14 Birth and death rates as functions of age x .

characterization is as shown in Figure 3.13. Note that we have different death rates for each group, and there is transition from group 1 to group 2 and from group 2 to group 3, and additions to group 1 with births. In the second, we characterize the age of each human continuously. In this case we have one single variable $N(t, x)$ with $N(t, x) \delta x$ representing the number of people in the age group x to $x + \delta x$ at time t . In this case the birth rate $b(x)$ and death rate $d(x)$ need to be specified as continuous functions of age. Typically the shapes of these functions are as shown in Figure 3.14. Death can occur at any stage, and this is reflected in the continuous distribution of death rate with age. Death rates are higher than average at very early ages (infant mortality) and at old age. In contrast, the birth rate is non-zero for a limited age range because of the limited fertility period of females and male juveniles and old males being incapable of reproduction.

Yet another system characterization is one where we have only a single variable, $N(t)$, to represent the total population at time t , but includes the gestation period. In this case we have an extra new parameter τ to represent this period, and the rate of change in $N(t)$ at time t depends on $N(t - \tau)$.

When we treat the time variable as discrete, the system is characterized by variables representing population numbers at discrete time instants. Changes to these variables occur due to births and deaths over the interval (Δ) between two successive discrete time instants. Thus, instead of birth and death rates (as in continuous time characterization) we have births and deaths over different intervals. In the simplest description we have, for each interval, three variables – $N(t)$, $B(t)$ and $D(t)$, with t representing the interval number; $N(t)$ the population at the end of the interval; $B(t)$ and $D(t)$ representing the births and deaths in the interval. The relationship between the variables is as shown in

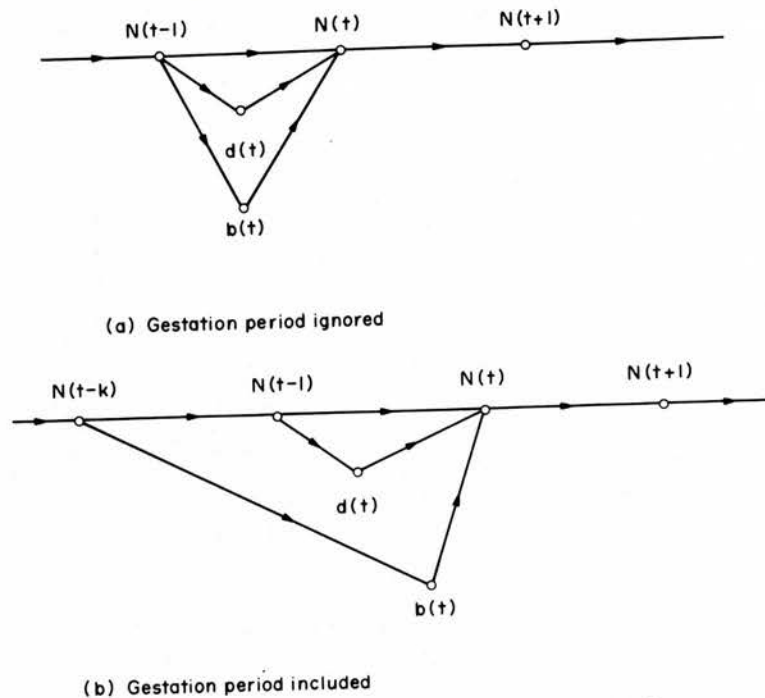


FIGURE 3.15 System characterization for Case Study E.

Figure 3.15, where the first characterization ignores gestation and the second includes it. (It is assumed that the interval length Δ and gestation period τ are constant with $\tau = k\Delta$.) We can obtain more detailed characterizations of the system using similar approaches to those above when time was taken as a continuous variable.

Comment. In the above system characterization we have assumed that the changes to the variables are predictable. This assumption is justified only when the population numbers are large and the interval of study is small. When one or both of these assumptions do not hold, then uncertainty becomes an important feature of the system characterization.

We have also assumed that the changes occur gradually in the case of continuous time characterization. This implies that it is inadequate to describe catastrophic changes that can occur due to large-scale disasters. We have also assumed that in the simplest characterization the parameters b , d and L are constants. This is valid if there are no external factors affecting them. If we assume that L depends on factors such as technology level, d depends on medical advances, etc., then we need to incorporate these into the system characterization. This can be done by regarding these as influences from outside the system (i.e. from the system environment) and treating the system

as an open one. This will result in more variables and a more refined description.

6.6 Case Study F [Cont.] (River Pollution)

In order to solve the problem of how to keep concentration levels of pollutants below prescribed levels, Gamma Inc. needs to obtain changes to concentration levels in the river over time under different dumping policies for chemical waste. A policy for dumping is defined by the time history of dumping.

We shall assume that the dumping is carried out at discrete time instants. The effect of dumping is to increase the concentration level suddenly, at the moment it occurs. With the passage of time the chemical waste diffuses into the water and also gets transported downstream. Depending on the waste, it can either go through a process of transformation so that it ceases to be an undesirable waste (as with biodegradable waste) or retain its chemical structure and continue to be an undesirable chemical waste.

In the systems approach the river can be treated as a single object with the waste dumped being an input variable (from the system environment) and the water discharged, either to an ocean or a lake, being an output variable (to the system environment). In the simplest characterization the river can be viewed as a one-dimensional channel, of constant cross-section A , with $x = 0$ corresponding to the location where the waste is dumped into the river. Let L_1 and L_2 represent the length of the river upstream and downstream from the point where the waste is dumped. As a result, we have $-L_1 < x < L_2$ with distances measured downstream being positive and those measured upstream being negative. The variable of interest is given by $T(t, x)$ – the concentration level of chemical waste at location x from the point of dumping at time t . The variable changes continuously with t and x . Another variable of interest is the velocity of flow – the simplest characterization for this is when it can be treated as constant of value U .

Since the river receives clean water from an external source the concentration level is zero at $x = -L_1$, hence $T(-L_1, t) = 0$. If we assume that the lake or ocean to which the river discharges is very big, then the concentration level there is also negligible. Hence $T(L_2, t) = 0$. The diffusion and transportation of the waste is predictable and governed by the laws of fluid mechanics.

As a consequence the problem can be described in terms of an open, deterministic dynamic system. The aim is to obtain time histories of concentration levels under different dumping policies so as to select the policy which disposes maximum waste without exceeding acceptable limits.

In the above characterization we have viewed the river as a one-dimensional channel with constant cross-section and ignored the lateral diffusion of the chemical waste across the width. Since the waste is dumped at a point, rather than along the whole cross-section, the above characterization is an oversimplification. A more refined characterization includes such spatial variations.

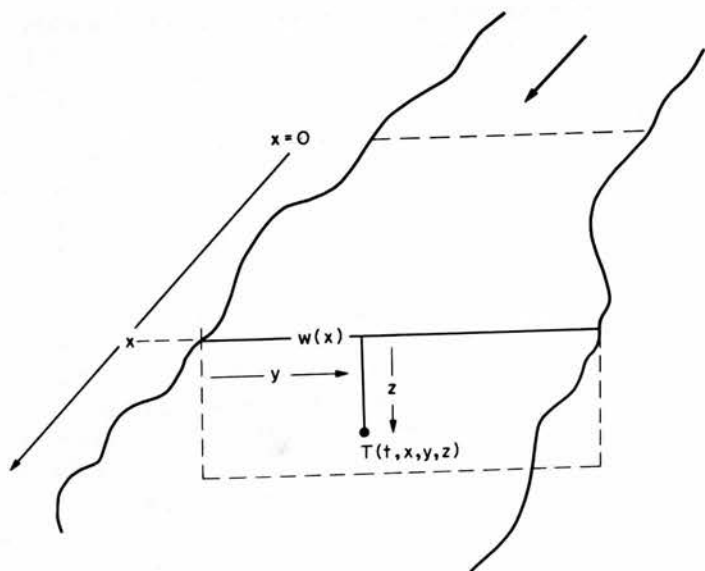


FIGURE 3.16 Coordinate frame for Case Study F.

For example we can treat the depth as being nearly constant (and represented by a parameter h) and the width of the river as changing with x . Let $w(x)$ represent the width of the river at a distance x from the point of dumping along the river, then the cross-sectional area $A(x)$ changes with x . The concentration level is given by a variable $T(t, x, y, z)$ – the concentration at a point whose coordinates are given by (x, y, z) (see Figure 3.16) at time t . The limits for x are as defined earlier; for y and z they are given by $0 < z < h$ and $0 < y < w(x)$. Since the flow volume must be constant for all x , the velocity of flow, $U(x)$, is a function of x .

There are many different time scales in this system characterization. We mention a few: (i) time for chemical reaction; (ii) time for diffusion; and (iii) time for transportation ($\sim L_1/U$).

Comment. If the river is discharging into an ocean and L_2 is small, then we need to incorporate the effects of tides. In this case we have another time scale associated with the occurrences of tides. We have also assumed that the river receives fresh water from a single source. A refined description would be needed if there is more than one source feeding the river. If the volume of flow changes considerably, then this must also be taken into account.

6.7 Case Study G [Cont.] (Weather Changes)

The economic viability of the solar heating system for a swimming pool depends on the number of days in a year it is sunny (i.e. sunshine for more than

8 hours) and partly sunny (i.e. sunshine between 4 and 8 hours). On these days there are savings to be made in the consumption of liquid fuel if a solar heating system is installed. The installation of such a system will be economically justifiable if these savings exceed the total of the operating and capital repayment costs. Thus the most critical variable in the economic analysis is the number of days in a year when it is either sunny or partly sunny. Hence we need to obtain estimates for the number of sunny and partly sunny days in a year.

Towards this end, we note that changes of weather over time are unpredictable and influenced by many factors. The time and length scales associated with these factors can vary considerably – ranging from a few minutes to days and from a few kilometres to thousands of them. Also, not all factors are properly understood. This suggests that a “black-box” representation may be appropriate with the description given in terms of a closed dynamic system with a high degree of uncertainty. Since our interest is in the number of hours of sunshine in each day, the time variable is best treated as being discrete with the interval of discretization being a day (from midnight to midnight). Let $N(t)$ represent the weather on day t , viz. sunny, partly sunny or cloudy. As a result we let $N(t)$ assume the following three values:

$$\begin{aligned} N(t) &= 1 \text{ if day } t \text{ is sunny,} \\ &= 2 \text{ if day } t \text{ is partly sunny,} \\ &= 3 \text{ if it is cloudy.} \end{aligned}$$

$N(t)$ changes randomly with time. Recognizing that there is a certain persistence about weather patterns, $N(t)$ at time t could be characterized as depending in a random manner on the value at $t-j$, i.e. $N(t-j)$, $1 < j < J$. Note that this ensures that the principle of causality is not violated. J is a parameter reflecting the degree of dependence on the past. J being large implies that the influence of factors with large time scales is included.

We shall assume that $J = 1$ for the simplest characterization. In this case we have the system parameters given by the probabilities characterizing the random transitions.

Comment. In the above characterization we assumed that the probabilities of transition do not change with time, and hence are treated as parameters. This assumption is often not justified. A slightly more refined characterization is to divide the year into different seasons – summer, winter, etc. – and use different probabilities of transition for each season.

6.8 Case Study H [Cont.] (Thermal Power Station)

The thermal power station produces electricity by burning coal. The process is not direct. The chemical energy in the coal is released as heat by combustion

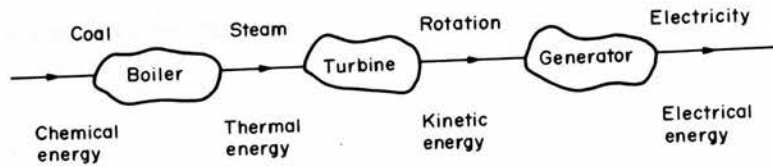


FIGURE 3.17 Energy transformation in a thermal power station.

and the heat in turn is used to convert water into steam. These two processes occur in the boiler. The steam produced in the boiler is fed into the turbine where the thermal energy in the steam is converted into rotational kinetic energy. This energy is used to drive the rotor of the generator and a rotating magnetic field is set up by exciting the rotor. When the magnetic field cuts the conductors of the stator, energy transfer occurs resulting in the kinetic energy being transformed into electrical energy. This sequence is shown schematically in Figure 3.17.

The voltage and frequency of the electrical output must always be held close to some pre-specified values. As the electrical load (i.e. demand) on the power station varies, the input to the boiler, turbine and generator must be varied so that the output of the generator matches the load. This is usually done by means of various regulators; the problem is to design these regulators. In order to do this one needs to understand how changes to input affect the output for the boiler, the turbine and the generator. We shall confine ourselves to studying these changes.

For the purposes in mind, the thermal power station can be viewed as a closed deterministic dynamic system consisting of three interacting subsystems with output from the boiler (first subsystem) being the input to the turbine (second subsystem) and the output of turbine being input to the generator (third subsystem).

In the simplest characterization each subsystem can be viewed as a "black box" with the input and output related by a dynamic relationship. The different input/output variables for the three subsystems are as shown in

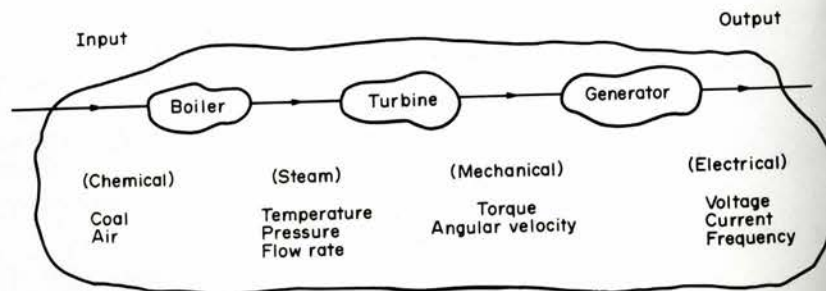


FIGURE 3.18 System characterization for Case Study H.

Figure 3.18. The goal of the study is to find the dynamic relationships linking the input to the output for each of the three subsystems.

Comment. Instead of viewing the subsystems as "black boxes" one can characterize each of them in terms of the physical processes taking place. This would lead to a more detailed description involving a large number of variables.

6.9 Case Study I [Cont.] (Component Reliability)

Since the control element is essential for the operation of the machine, the machine becomes inoperable whenever the element fails, and is made operable by replacing the failed element with a new working one. The solution to specific problems regarding the operation of the machine can be obtained by focusing attention on the control element.

A description of the control element, in the context of the problem, can be done in terms of an open system with a single object and a system environment as shown in Figure 3.19. The simplest characterization, using the "black box" approach, involves a single variable, $X(t)$ with

$$X(t) = 1 \text{ if the element is working at time } t, \\ = 0 \text{ if the element is not working at time } t.$$

Thus, $X(t)$ changes from 1 to 0 whenever a failure occurs, and from 0 to 1 whenever a failed element is replaced by a new one.

Let τ_i , $i = 1, 2, \dots$ represent the time to failure (or age at failure) for the i th element. τ_i is a random variable. If all spares are identical and failures are independent, then the various times to failure are a sequence of independent and identically distributed random variables. Let ρ represent the time needed

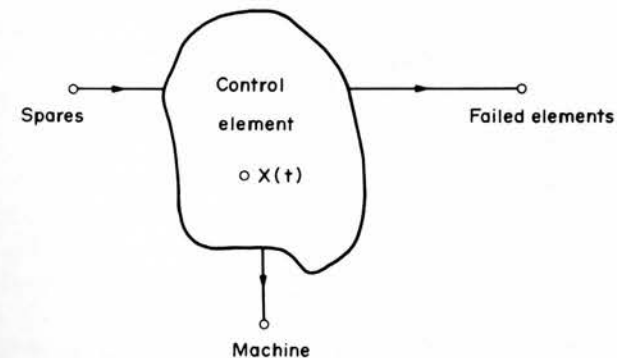
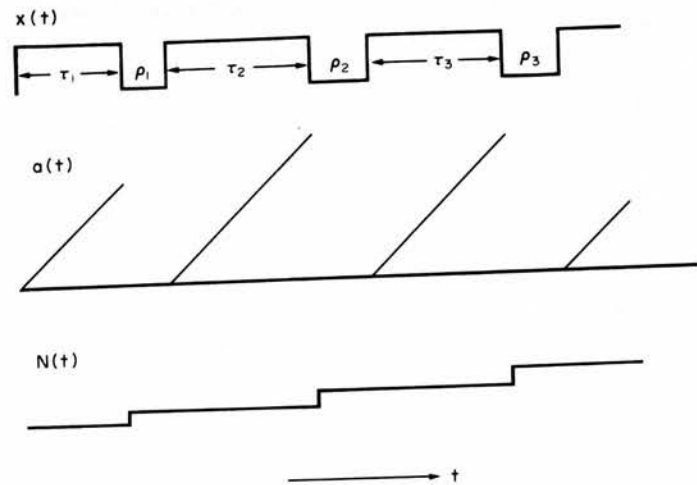


FIGURE 3.19 System characterization for Case Study I.

FIGURE 3.20 Time histories of $X(t)$, $a(t)$ and $N(t)$ for Case Study I.

to replace a failed element by a new one. We assume that there is very little variability associated with this, and hence it can be treated as a constant.

If we assume that the state is continuously monitored, then failure is detected at the instant it occurs. We assume that replacement commences immediately after an element fails. Then $X(t)$ changes randomly over time. Let $N(t)$ represent the number of replacements that have taken place in the interval $[0, t]^*$ and $a(t)$ be the age of the element at time t if $X(t) = 1$. A typical history of $X(t)$, $N(t)$ and $a(t)$ is as shown in Figure 3.20.

If ρ is small in relation to the mean life of the control element, then we can approximate ρ as being zero. This is a simplification which is valid in many instances. In this case the instances of failure (as well as replacement) can be regarded as random points along time, with the time interval between successive points corresponding to failure times of different spares.

The system parameters are the parameters of the distribution function characterizing the time to failure; T the total time interval of interest and NT the total number of spares available.

An alternative characterization (as opposed to the previous "black-box" characterization) is one which describes the mechanism of failure of the element. Suppose that failure occurs due to crack propagation. In this case the variables characterizing the system are given by $X(t)$ and $Y(t)$. $X(t)$ is as defined earlier; $Y(t)$ represents the crack length at time t if $X(t) = 1$. If $X(t) = 0$ then $Y(t)$ is not defined; $Y(t) = 0$ at the instants at which the replacement of a failed element is

*Note that here and subsequently we are using standard mathematical bracket conventions that square brackets $[a, b]$ denote a range of values including a and b whereas parentheses (a, b) denote a range within a and b .

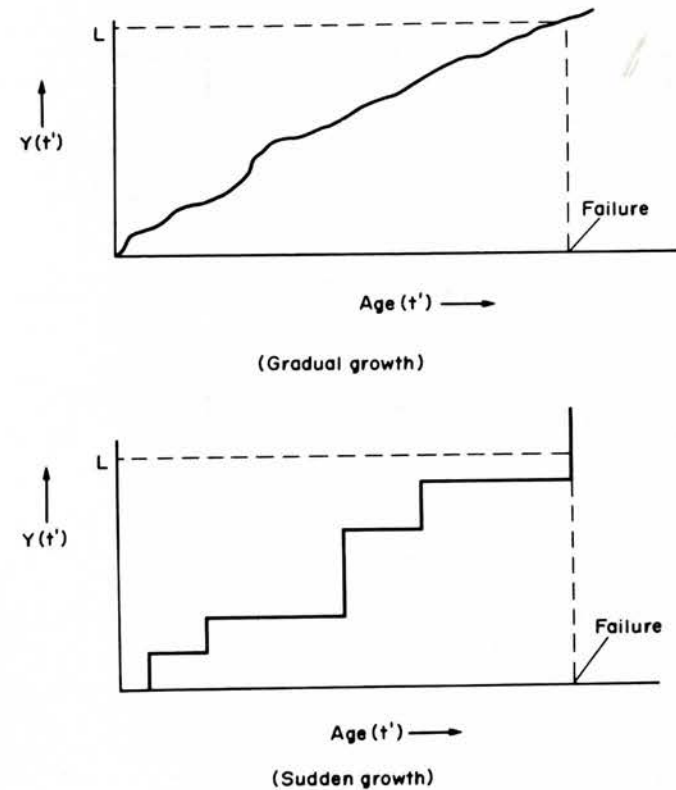


FIGURE 3.21 Crack propagation for Case Study I.

completed and the machine made operational. Failure occurs when $Y(t)$ reaches some critical value L . The crack propagates randomly with time and the changes over time can be either as gradual or sudden as indicated in Figure 3.21. The latter characterization is appropriate if the growth in crack occurs due to shocks occurring randomly in time and the effect of each shock on crack growth is random.

The goal of this study is to obtain the statistical characterization of: (i) the instant at which the last spare fails and (ii) the number of spares, $N(T)$, needed to keep the system operational for a period T .

6.10 Case Study J [Cont.] (Speed of Aeroplanes)

The problem is to forecast the maximum speed of aircraft in the year 2000. Improvements to the maximum speed of aircraft occur with advances in technology. The processes responsible for these changes are very complicated and involve many factors.

We can describe the changes to maximum speed of aeroplanes in terms of a

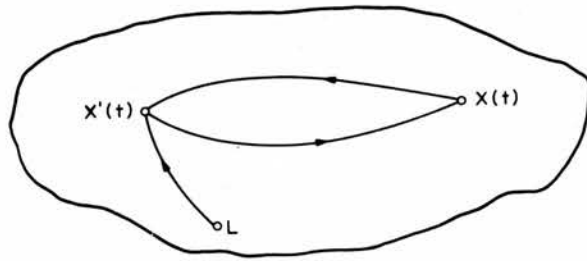


FIGURE 3.22 System characterization for Case Study J.

closed system. The simplest characterization, based on a “black-box” approach, involves a single variable, $X(t)$, representing the maximum speed achieved at time t and increasing with time in a deterministic manner. One can characterize this increase over time in two different ways:

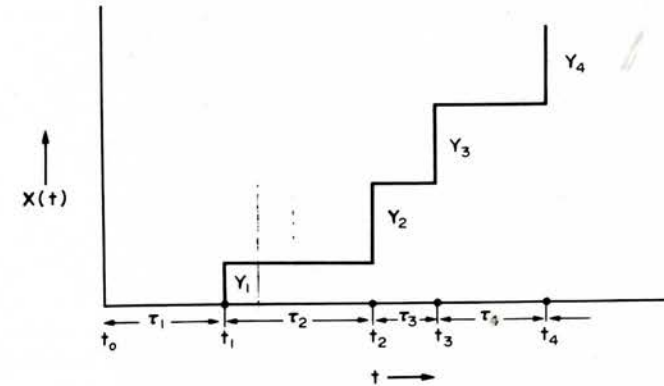
- (i) $X(t)$ changes according to some pre-specified function $D(t, \theta)$ with θ being a set of parameters, or
- (ii) $X'(t) \{ = dX(t)/dt \}$ being influenced by $X(t)$ in some pre-specified manner as shown in Figure 3.22, with L , a parameter, representing the upper limit to the maximum speed.

In real life, technological changes occur in an unpredictable manner and hence the assumption that changes to the maximum speed are deterministic is obviously inappropriate. A way of incorporating the uncertainty is to view the speed achieved at time t being of the form

$$X(t) = D(t, \theta) + V(t)$$

where $D(t, \theta)$ is a deterministic function and $V(t)$ is a stochastic process reflecting uncertainty.

An alternative characterization is as follows. Technological changes do not occur continuously in time – rather, they occur at discrete time instants due to technological breakthroughs. The time instants of breakthroughs, as well as the effect of each breakthrough on the speed, are highly variable and hence need to be characterized in a stochastic framework. Let t_i denote the time instant at which the i th breakthrough occurs and let Y_i represent the improvement in the maximum speed due to the breakthrough. $X(t)$ is a cumulative sum of breakthroughs and a typical plot of $X(t)$ is shown in Figure 3.23. Let $\tau_i = t_i - t_{i-1}$, $i = 1, 2, \dots$ and with $t_0 = 0$. Then, τ_i , $i \geq 1$, represents the time interval between two successive breakthroughs and is a sequence of random variables. Let $N(t)$ represent the number of breakthroughs in the interval $[t_0, t]$ and this is also a random variable. We assume that Y_i is a sequence of independent and identically distributed random variables with a distribution function $F(\cdot)$ and that τ_i is also a sequence of independent and identically distributed random variables with a distribution function $G(\cdot)$.

FIGURE 3.23 Typical plot of $X(t)$ for Case Study J.

Comment. In the simpler characterization we have assumed L to be a constant. The value of L depends on the type of technology. In the case of aeroplanes we have three distinctly different technologies – propeller-driven engines, jet engines and rockets. Thus a more refined characterization is one where we have three different limits – L_1 for the propeller; L_2 for the jet and L_3 for the rocket with $L_1 < L_2 < L_3$. The older technology gets replaced when a major technological advance occurs. These changes need to be characterized. Within a given technology type, changes occur as described earlier. A similar refinement can be done for the alternative stochastic characterization. This can be done by separating breakthroughs into two types – major and minor. Major technological breakthroughs result in a change in the technology type whereas minor breakthroughs result only in speed improvements within the current technology.

6.11 Case Study K [Cont.] (Supermarket Operation)

Here we are interested in determining the optimum number of checkout counters in a supermarket to maximize the expected profit. Queue lengths at checkout counters in a supermarket vary randomly over time. If there are insufficient checkout counters, queue lengths tend to be excessively long and this affects customer patronage. On the other hand, if there are too many counters the operating costs are increased. In either case the profitability of the supermarket is affected. Thus a suitable trade-off must be made between the number of counters installed and customer patronage to maximize profits. In other words, the problem is solved once a relationship between some measure of queue (e.g. average queue length or average time period for which the customer has to wait before being served) and the number of checkout counters is obtained.

Towards this end, the problem can be described as an open dynamic system. The variables characterizing the system are $N(t)$, the number of customers either in the queue or being served, and M , the number of checkout counters. $N(t)$ changes randomly with time. It increases whenever a customer joins the queue and decreases whenever a customer leaves after being served. The system characterization is shown in Figure 3.24. We treat the time variable as being continuous. We assume that customers arrive randomly and also that the time to serve a customer is random. In the simplest characterization we assume that the inter-arrival times are independent and identically distributed with a distribution function $F(\cdot)$ and that the service times are also a sequence of independent and identically distributed random variables with a distribution function $G(\cdot)$. We assume that an entering customer joins the shortest queue and does not change queues during the waiting time.

The goal is to obtain the expected queue length as a function of the number of checkout counters.

Comment. A more refined characterization is one where the checkout counters are divided into "normal" and "fast". Customers with more than L items can be served only at a "normal" counter, while those with less than or equal to L items can be served at either of the counters. The assumption that queue changing is not allowed is also often inappropriate. This can be overcome by allowing customers to change queues based on some rational rule – e.g. as the adjacent queue becomes shorter there is a possibility for a customer to change queues.

In the simplest characterization we have assumed that the inter-arrival times are identically distributed. A refined description would drop this assumption and allow the distribution to change with the time of the day. This would account for busy and slack periods of shopping. A still more detailed description would take into account factors such as special sales, influence of advertising, etc.

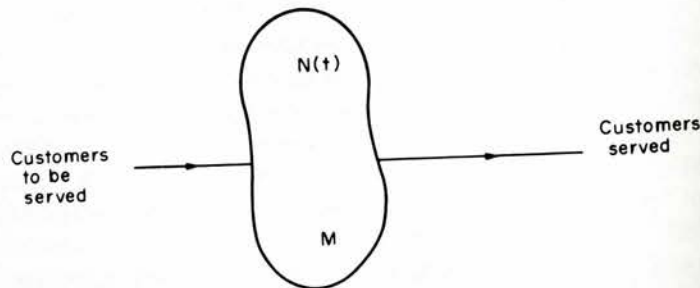


FIGURE 3.24 System characterization for Case Study K.

6.12 Case Study L [Cont.] (Demand for Soft Drinks)

The demand for soft drinks varies with time and is influenced by many factors – price, advertising, competition, population changes, seasonal variations, taste, conditioning, etc. The effect of some these factors on the demand is predictable, but for most it is uncertain.

Since the demand changes dynamically, the time variable is important and can be treated as being either continuous or discrete. Discrete time characterization is more appropriate, for then we can characterize the problem in terms of demand over different time intervals or periods. A month is a convenient interval to use for characterization, since seasonal variations can then be easily included in the characterization. A weekly description is too detailed whilst a yearly description is too coarse.

The simplest characterization can be done in terms of a closed dynamic system involving a single variable, $X(t)$, representing the demand for the soft drink in period t , and being composed of two terms:

$$X(t) = D(t) + V(t)$$

where $D(t)$ is the deterministic part representing the effect of factors whose influence is predictable (e.g. growth in population, seasonal variations) and $V(t)$ the stochastic part representing the effect of factors whose influence is uncertain. Because of the dynamic nature of change, $D(t)$ is a function of its past values and, similarly, $V(t)$ is a function of its past values. As a result we can view $X(t)$ as a function of its past values and of $D(t)$ and $V(t)$ and possibly their past values. Since there is yet no theory to characterize the relationships, they must be obtained empirically using the historical data given in Table 2.7.

The goal of the study is to obtain this relationship, and once this is done the demand in the future can be forecast.

Comment. In the above characterization the effect of the different factors is either ignored or included in an implicit manner. An alternative characterization is one where the effects of these factors are described explicitly. In this case the problem can be described in terms of an open system with the relevant factors as inputs from the environment. The characterization will be more involved – e.g. advertising can affect the behaviour of a competitor, which in turn alters the effectiveness of the advertising and so on. This illustrates the statement made in an earlier section that identifying causal relationships between variables in social/economic systems is in general a difficult task.

Notes and References

Over the past few decades a large number of books have appeared on systems thinking and the systems approach. Items [1]–[8] are a small sample; a more philosophical approach can be found in [9]–[11].

Similarly, the number of articles on system concepts and methodologies that has appeared, and continue to appear, in various journals is also very large; [12] and [13] are two examples.

The concepts (discrete vs continuous time, causality, understanding of subsystems, etc.) discussed in this chapter have deep implications at practical as well as philosophical levels. For further discussions on these issues see [14]–[16] and other articles that have appeared in various philosophical journals and system theory journals.

A good discussion of graph-theoretical methods for representing system characterization can be found in [17]. Bond graph is a special type of representation useful for characterizing electrical, mechanical and pneumatic systems. The details of this type of representation and its use in representing other types of systems can be found in [18]. For other types of representation such as matrix tabular representations, signal flow diagrams, see [19] and [20].

[21]–[31] are a small sample of books which illustrate the growing use of the systems approach in understanding and in solving problems from a diverse range of disciplines.

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CHAPTER 4

Mathematical Modelling

1 Introduction

In the previous chapter we showed that the process of solving a real-world problem can be treated as the study of a system with a defined goal. In this chapter we discuss the modelling of such a system. We commence with a brief discussion of models in general so as to define the sense in which we use the word "model" in this book. Following this, we discuss the different types of models and examine a particular one – the mathematical model – in some depth.

Our main aim in this chapter is to develop the process of mathematical modelling in which a physical system is translated into a mathematical description. We do this by first presenting a simplified version which illustrates the main steps of the modelling process. Later we present a more detailed version which highlights the identity and role of the many different topics required for successful modelling.

2 A General Introduction to Models*

2.1 Model-Varying Meanings

One of the major deficiencies of most natural languages is that the same word is often used to convey different meanings and concepts. The accepted meaning, in the "everyday sense", depends to a large extent on the context in which it is used. In the case of the word "model", an examination of any good dictionary reveals that its usage is large and varied. It is used both as a noun and as a verb. In well-developed branches of learning (e.g. physics, logic, engineering), words are used in a more precise or definite sense – a "technical sense", as opposed to an "everyday sense". Even in the "technical sense" there is no single accepted meaning of the word "model". Its meaning varies from one branch of learning to another, as illustrated by the following quotations.

*Sections 2–5 can be skipped when reading for the first time, as they deal with broader (and philosophical) issues of models and modelling.

- (i) *Mathematical logic*. "A possible realization in which all valid sentences of a theory T are satisfied is called a model of T " (Tarski [20]).
- (ii) *Physics*. "... the proposition comprising a model of an X are the same as ones constituting what may be called a theory of an X (The Bohr Theory of the Hydrogen atom)" (Achinstein [21]).

Although the word model used here has a precise and well-defined meaning in each branch of learning, the meaning is different in each usage. Thus, it is essential to state clearly the usage intended in a particular context so as to avoid any confusion.

2.2 "Model" as used in this Book

Our usage of the word "model" in this book is given by the following definition – "A model is a representation of a system." Furthermore, a "model" is said to be an "adequate model" if it is adequate for the goal in the mind of the modeller.

The key terms in the above definition are: (i) system, (ii) representation, (iii) goal, and (iv) adequate. We need to define these terms so as to give a precise meaning to our usage of the word "model". We have discussed "system" and "goal" in Chapter 3. In this section we explain the remaining two terms.

2.3 Representation

A representation of a system, in general, contains less information than the system it represents. This point is important, as the representation should contain only those features or characteristics of the system which the model builder feels are relevant and significant for the goal in mind. The representation of a system can be either a physical device or an abstract formulation. A few examples of the different types of representations are:

(i) SCALED REPRESENTATION

Here the physical object is represented by a scaled-down version in which some scaling relationship is obeyed. For example, a geometrically similar scaled model of a building may be used in a wind tunnel with the goal of predicting wind loads on the real building.

(ii) PICTORIAL REPRESENTATION

Simple examples include a globe representing the earth, a map representing topographic features of the land surface or a photograph representing some physical object.

(iii) VERBAL REPRESENTATION

This consists of a verbal description of a system in one of the many man-made languages such as English. For example, the description of an elephant in terms of its physical characteristics such as size, colour, shape and so on.

(iv) FIGURATIVE/SCHEMATIC REPRESENTATION

One simple example of this is the ball-and-spoke representation of a complex molecule in which the balls represent atoms and the spokes interatomic bonds. Another is a schematic representation of an electrical network in which the physical objects in the network, such as resistor, capacitor and so on, and their interrelationships, are represented by connected symbols.

(v) SYMBOLIC REPRESENTATION

In this the system is represented by a formulation involving symbols. The symbols have well-defined meanings and can be manipulated according to some set rules. For a symbolic formulation to become a representation of a system, a one-to-one correspondence must be established between the symbols of the formulation and the physical features or characteristics of the system. Without this correspondence the symbolic representation is abstract.

2.4 Adequacy

The system under study is usually complex. The model is a representation which is simpler and, hopefully, at the same time adequate. The process of simplification is justified, because only some features of the system are significant for the goal of the study. This was discussed in the previous chapter and we illustrate it again by the following example.

Example 1

The colour of a car or the type of upholstery is not significant for a study of the ride characteristics of a car.

In building a model of a system one should take a pluralistic view of the system by realizing that it can have multiple representations. Hence, *model building can be viewed as the process of selecting an appropriate and adequate representation.*

This raises the question of when a representation is adequate. This is a difficult question to answer, for it involves many conflicting factors and we shall defer discussion of this aspect to a later chapter.

3 Model Classification

Broadly speaking, models can be classified into two main types or categories:

- (1) material or physical models;
- (2) non-material or formal models.

As the name suggests, material models have a physical existence with a direct relation to the real-world problem. For example, a *scaled model* of a system is a replica of that system, and is related to the original system through a scale transformation in terms of features that are important. In many cases it is not possible to build a scaled model; for example we cannot build a scaled model of the planetary system and of the rocket to see if the rocket will perform satisfactorily.

In contrast, non-material or formal models are abstract representations. These may take a physical form, such as symbols written on a sheet of paper, but have no direct similarity with the real-world problem. For example, a *descriptive model* of a system is a representation of the system in some natural language. We have already encountered one such representation – termed “system characterization” – in the previous chapter. A system characterization is a descriptive model of the system associated with the problem, and plays a very important role in building a mathematical model.

Later in this chapter we will briefly examine types of models which have an important relation to mathematical models.

4 Mathematical Model

A mathematical model of a system is a symbolic representation involving an abstract mathematical formulation. A mathematical formulation is composed of symbols, and makes no sense outside mathematics. The symbols have precise mathematical meaning and the manipulation of symbols is dictated by the rules of logic and mathematics. A mathematical formulation is not a model by itself. It is only by relating the mathematical formulation to a system characterization (i.e. variables and relationships, as discussed in the previous chapter) that the formulation becomes a mathematical model. An *adequate mathematical model* is a mathematical model which is adequate for the purpose in the mind of the builder.

Example 2 (World Population: Case Study E)

The following first-order ordinary differential equation formulation

$$dn(t)/dt = a\{L - n(t)\}$$

with $n(t_0) = n_0$ specified, is an abstract formulation which makes no sense outside mathematics.

By associating the variables $\{t, n(t)\}$ and the parameters $\{a, L\}$ of the formulation, on a one-to-one basis, with the variables and parameters of a system characterization, as indicated below, the above formulation becomes a mathematical model for population changes:

Formation	System characterization
t	Time
$n(t)$	Population at time t
a	(Birth rate)—(Death rate)
L	Limit on population

A different way of looking at this is to view the abstract mathematical

formulation as a dummy which makes no sense outside mathematics. By clothing it properly, i.e. by associating the symbols of the formulation with the variables of the system characterization, we convert the dummy into a mathematical model.

4.1 Empirical vs Theoretical Model

The selection of a suitable mathematical formulation to serve as a dummy, which results in a mathematical model after proper clothing, is far from trivial. If the system characterization is done using terms from well-established theories, the selection of an appropriate formulation to serve as a dummy is relatively easy, for it will follow from the mathematical laws associated with those theories. Models in this category are sometimes called "theoretical models".

If, on the other hand, a system characterization is based on no theory or knowledge, as in the case with systems viewed as "black boxes", the mathematical formulation to serve as a dummy must be selected on an ad-hoc basis. Models in this category are sometimes called "empirical models".

In this book we will not differentiate between theoretical and empirical mathematical models, but simply call all of them "mathematical models".

4.2 Classification of Mathematical Models

Mathematical models can be classified into four categories based on the mathematical structure of the underlying formulation. The four categories are as follows:

- Category A: formulations suitable for modelling deterministic static systems.
- Category B: formulations suitable for modelling deterministic dynamic systems.
- Category C: formulations suitable for modelling probabilistic static systems.
- Category D: formulations suitable for modelling stochastic dynamic systems.

Each of these categories can be further subdivided. We discuss formulations belonging to categories A and B in Chapter 5, and to categories C and D in Chapter 7.

5 Analog and Simulation Models

5.1 Analog Models

Analog models are material (or physical) models which are used extensively in many branches of learning. An analog model can be formally defined as

follows: "A real system S_1 is an analog model of another real system S_2 (or vice-versa) if and only if the mathematical models of the two are identical in terms of the mathematical formulation used to build the models." This implies that there exists a one-to-one correspondence between the variables of the system characterization of S_1 and S_2 . We give a simple example of illustrate this.

Example 3

A mechanical system can be characterized in terms of objects such as masses, springs and dashpots, using variables such as force, displacement, mass, spring stiffness and damping. Using the well-known laws of dynamics we can obtain a mathematical model involving an ordinary differential equation formulation as a dummy. An electrical network consisting of capacitors, inductors and resistors can be built such that the resulting mathematical model uses the same ordinary differential equation formulation as a dummy. In this case, each is an analog (model) of the other, and there is a one-to-one correspondence between the variables as indicated below:

Mechanical system		Electrical network
Force	$\leftrightarrow$	Voltage
Displacement	$\leftrightarrow$	Charge
Mass	$\leftrightarrow$	Inductance
Spring stiffness	$\leftrightarrow$	Capacitance
Damping	$\leftrightarrow$	Resistance

It is important to note that the validity of S_1 and S_2 as analogs of each other is often true only under certain conditions. In the above example the analogy is valid only at low frequencies.

5.2 Simulation Models

A simulation model of a system is another system that imitates the latter in some respect, such as in shape or function.

Since the goal is to simulate only *certain aspects* of the given system, the building of a simulation model often requires only a scant knowledge of the system being simulated, as illustrated by the following example.

Example 4

A quartz mercury lamp simulates the sun, in the sense that spectra of the two are similar.

Simulation is a crude and deliberate imitation. It is dictated more by pragmatic considerations. Thus a simulation model of the kind described above contains less information of the system than an analog or a mathematical model of the system.

With the advent of computers the term "simulation" has acquired a special meaning, for in that context it refers to the relationship between a mathematical model and its implementation on a computer, as shown in Figure 4.1. In this usage, "simulation" is a relationship that concerns the faithfulness with which the computer carries out the instructions intended by the mathematical model. In executing these instructions it is mimicking the system. This topic is discussed in detail in Chapter 9.

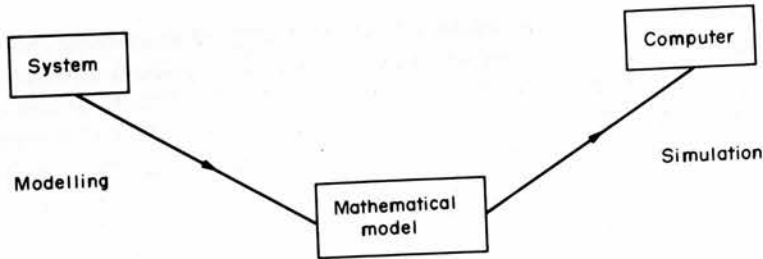


FIGURE 4.1 Model/modelling/simulation.

6 Mathematical Modelling

As indicated earlier, an adequate mathematical model of a system is obtained by relating, on a one-to-one basis, the features of an adequate system characterization with the variables of an appropriate mathematical formulation.

In general, one seldom obtains an adequate mathematical model at the very first attempt. This is because either the system characterization is not adequate or the mathematical formulation is not appropriate. This implies that an iterative procedure is needed, where at each stage an improved model is built and tested for adequacy. If it passes the test the model can then be said to be an adequate model; if not, the iterative process is continued.

There is yet no theory of mathematical modelling, and it is difficult to envisage the evolution of such a theory in the near future. Each new modelling exercise poses new challenges. This does not imply that there is no procedure for mathematical model building. In fact there is a basic methodology which is common to all mathematical modelling exercises. We shall first present a simplified description of the mathematical modelling process to illustrate the main steps. This is followed by a more detailed description which highlights the different topics needed for modelling.

6.1 Mathematical Modelling Process (Simplified)

The mathematical model building process, in the simplest form, can be viewed as an iterative multistep process as shown in Figure 4.2. It consists of four steps, and we briefly discuss each of them.

Step 1 (System characterization). This was examined in the previous chapter and can be viewed as a process of simplification and idealization. The execution of this stage requires a deep understanding of the physical aspects of the system (associated with the real world of the problem).

Step 2 (Mathematical model). This involves two stages. In the first stage a mathematical formulation is selected. The type of formulation selected is

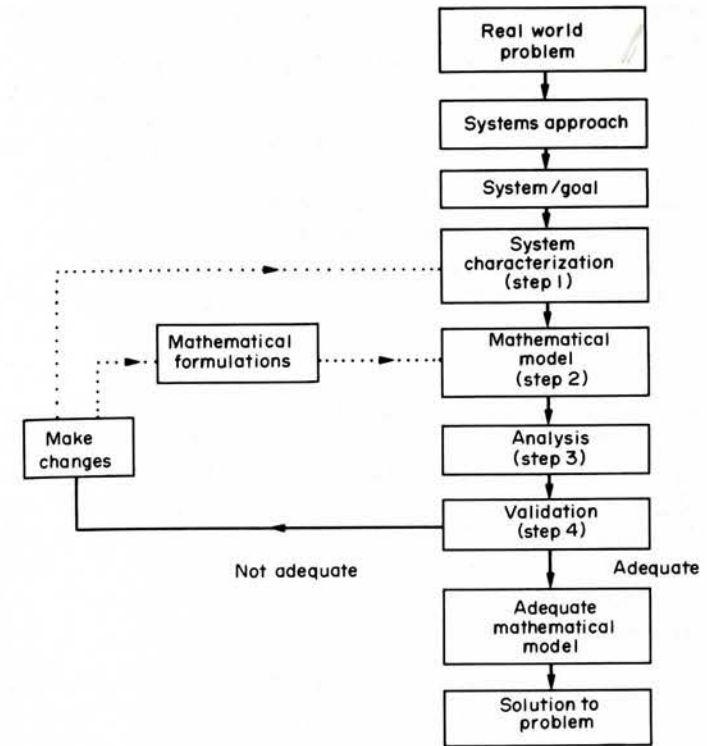


FIGURE 4.2 Mathematical modelling process (simplified).

sometimes dictated by the theory used in the system characterization, and when no such theory exists it is selected on an ad-hoc basis (i.e. based on the model builder's intuition). In the second stage the variables of the formulation are related on a one-to-one basis with the variables of the system characterization. Thus the "dummy" (abstract formulation) is clothed in terms of the physical features to produce a mathematical model. This step involves strong interaction between the physical aspects of the system (associated with the real world of the problem) and the abstract world of the mathematical formulation.

Step 3 (Analysis). In this, the relationship between the mathematical formulation and the system characterization established in Step 2 is temporarily discarded. This is because physical aspects of the system play no role in the analysis of the formulation. The analysis is abstract, and done according to the rules of mathematics.

Step 4 (Validation). In this, the analysis of the formulation is interpreted in terms of the relationship established in Step 2 (and temporarily discarded in Step 3) to yield the behaviour of the mathematical model. This behaviour is

compared with the behaviour of the system (equivalently, the data from the real world) to determine whether the two are in reasonable agreement according to some pre-defined criterion. This is called validation.

If the model fails the validation test it is inadequate for the goal in mind, and must be rejected. When such a situation occurs, one needs to back-track and make changes – either in the system characterization, the mathematical formulation selected or both. The changes must be done judiciously so that the new model is an improvement over that rejected. This iterative process is indicated by dotted feedback lines in Figure 4.2. The model building exercise comes to an end when the model passes the validation and the model becomes an adequate mathematical model.

(Note: The model building process stops once an adequate model is obtained. Since the aim is to obtain the solution to the original problem we need to execute the additional step shown in the diagram. This again illustrates that mathematical modelling is only a tool for solving real-world problems and not an end in itself.)

6.2 Validation Criterion

As discussed above, a model is accepted as an adequate model only when it passes the validation test. The test requires some criterion which can be used to compare the behaviour of the model with that of the system.

If the criterion specified is too stringent (i.e. it requires a very high level of agreement between the model and the system) then the resulting model will be complex. This follows since a detailed system characterization and a complicated mathematical formulation will be needed to produce an adequate model. On the other hand, if the criterion specified is not stringent, a model built on a coarser system characterization and involving a simple mathematical formulation may produce an adequate model. A stringent validation criterion results in the model and system behaviour matching in detail, but this is obtained at the cost of model complexity. An important aspect of model building is the selection of a suitable validation criterion which achieves a suitable trade-off between the degree of agreement between the system and the model and the complexity of the model.

One starts with a fairly stringent criterion and the simplest system characterization and mathematical formulation. Based on the degree of disagreement between the model and the system behaviour, either the criterion must be weakened or the model made more complex so that the two responses are closer in agreement. At the same time a critical evaluation must be made of the increase in the complexity and the cost-effectiveness in terms of time and effort needed to complete the modelling exercise. This is important, as time and effort are two factors that cannot be overlooked. This point again stresses

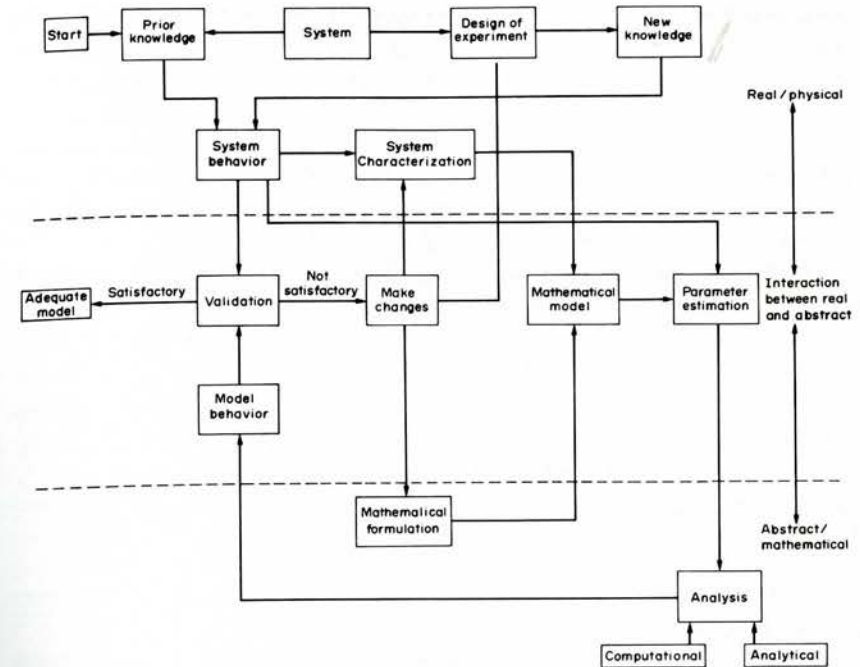


FIGURE 4.3 The model building process (detailed).

the art aspect of modelling, which requires critical evaluation and decision making.

6.3 Mathematical Modelling Process (Detailed)

The modelling process shown in Figure 4.2 does not illustrate all the features of mathematical modelling. Figure 4.3 shows the modelling process in greater detail. It shows more completely the different activities needed for successful modelling. It also shows the demarcation between the physical world of the system and the abstract world of the formulation and the interaction between the two. In this section we describe the modelling process shown in Figure 4.3, and comment on the different topics identified there.

The starting point is the real-world problem as indicated in Chapter 2. The problem is then transformed into a study of a system with the goal of the study defined. Describing the system, based on prior knowledge of its behaviour, produces the initial system characterization. This topic was discussed in detail in Chapter 3.

Relating the system characterization to a mathematical formulation produces a mathematical model. To do this one needs an understanding of the different types of formulation available. We discuss mathematical formul-

ations suitable for modelling deterministic systems in Chapter 5, and for modelling stochastic systems in Chapter 7.

In order to obtain the behaviour of the mathematical model one needs to assign numerical values to the parameters of the model. This is done by using system behaviour data (or data from the real world) in a process called "parameter estimation". This topic is covered in Chapter 10 both for deterministic and stochastic models. Once this is done the model behaviour can be obtained by the techniques of analysis.

The analysis depends on the structure of the formulation used in the model. Broadly speaking the analysis can be divided into two types – analytical and computational. To carry out the analysis one can ignore the correspondence between the formulation and the system characterization as the analysis is done in the abstract world of mathematics. In Chapters 6 and 8 we examine the analysis of formulations discussed in Chapters 5 and 7 respectively; in Chapter 9 we discuss the topic of simulation.

Often, prior knowledge is not sufficient to carry out the system characterization and/or parameter estimation. In such a situation one has to design an experiment to obtain new (or additional) knowledge. In Chapter 11 we discuss the design of experiments for system characterization and the parameter estimation.

Once the model behaviour is obtained it can be compared with the system behaviour (or real-world data) to assess the adequacy of the model. This is called validation, and this topic is considered in Chapter 12.

The solution to the original problem is finally obtained by carrying out an analysis of the adequate mathematical model and properly interpreting the results of the analysis.

Notes and References

No two definitions of the word "model" are identical. For a discussion on this issue see [1]. As mentioned in the text, the role and usage of models is varied. Item [2] is a collection of articles dealing with this aspect. In particular, the article by Suppes [3] examines critically the meaning and usage of models in different disciplines. Other articles of interest are [4]–[9]. An interesting book which deals with models in a wide framework is [10].

A variety of classifications for models have been proposed, see [11]–[13]. For more on analogies and analog models see [14]–[17]; on simulation and simulation models, see Notes and References at the end of Chapter 9.

Most books on mathematical modelling contain a fairly detailed description of models and modelling. For a fairly comprehensive list of such books see Chapter 18. In addition, many books dealing with specific topics (engineering, biology, operations research, etc.) contain a chapter or more on mathematical models and modelling – for example, [18] and [19] are two such books.

There are a large number of journal articles on mathematical models,

modelling and the teaching of modelling. Chapter 18 contains a list of such articles. Articles on modelling differ in presentation but the underlying methodology is more or less the same. In contrast, the methods advocated for the teaching of mathematical modelling are greatly varied.

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Mathematical Formulations – I

1 Introduction

In the previous chapter we described the different steps in the modelling process. The first step, system characterization, was discussed in Chapter 3. In this chapter we concentrate on the second step in the modelling process – relating the system characterization to a suitable abstract mathematical formulation. In order to carry out this step one needs a good understanding of the different types of mathematical formulations available, and a high level of skill in selecting the most appropriate formulation and relating it to the system characterization. This latter aspect is important, for often one can choose more than one type of formulation to serve as a dummy in modelling a given system.

We commence with a brief discussion of the different types of mathematical formulations that are suited for modelling deterministic systems – i.e. systems where uncertainty is not significant. Following this we examine five different types of formulations separately. For each formulation we give a brief introduction to the general structure, discuss some relevant aspects and finally illustrate their use as dummies in modelling one or more of the Case Studies A–L discussed in Chapter 2, using the system characterization given for each in Chapter 3.

2 Classification of Mathematical Formulations

Broadly speaking, the mathematical formulations suited for modelling deterministic systems can be divided into two categories: static formulations and dynamic formulations.

2.1 Static Formulations

Static formulations are mathematical formulations involving either algebraic equations or function optimization with one or more variables. The variables can be either scalars or vectors, either discretely or continuously valued and either constrained or unconstrained. When the formulation becomes a mathematical model there is a one-to-one correspondence between the

variables of the formulation and the physical variables of the system characterization. Such formulations are suited to modelling deterministic static systems.

2.2 Dynamic Formulations

Dynamic formulations involve two types of variables – dependent variables and independent variables. In the simplest type formulation there is only one independent variable and the dependent variables are functions of it. When the formulation becomes a model the independent variable is called time, and is denoted by t . The formulations are characterized by equations involving either the derivatives of the dependent variables with respect to time (when time is considered to assume a continuous range of values) or the dependent variables for more than one discrete value of time (when time assumes only discrete values).

More complex formulations involve two or more independent variables. The formulation is characterized by equations involving either the partial derivatives of the dependent variables with respect to these variables or the dependent variables for more than one set of discrete values of these, depending on whether the independent variables are treated continuously or discretely. In formulations involving four independent variables the independent variables are usually denoted by t , x , y and z . When the formulation becomes a model, t corresponds to time and the remaining independent variables correspond, say, to Cartesian spatial coordinates of the system characterization and there is a one-to-one correspondence between the dependent variables of the formulation and the physical variables of the system characterization.

Based on the nature and the number of independent variables in the formulation, we can divide dynamic formulations into four types, as indicated below:

Number of independent variables	Nature of independent variable	
	Discrete	Continuous
= 1	B1	B2
> 1	B3	B4

2.3 Formulation B1

In this formulation the dependent variables are functions of one independent variable (t) which takes on only discrete values: $t_1, t_2, \dots, t_i, \dots$. Without loss of

generality we can assume (by suitable scaling) that t assumes only integer values. Thus the independent variable $x(t)$ can be viewed as an indexed sequence $x(i)$ or x_i , with i taking on integer values. Formulations of this type are given by equations involving x_{n-i} , $0 \leq i \leq m$, and are called difference equation formulations. Such formulations are suited for modelling systems with discrete time characterization.

2.4 Formulation B2

In this formulation the dependent variables are continuous functions of the independent variable (t) which takes on a continuous range of values. Formulations belonging to this category can be divided into three types:

- (1) *Ordinary differential equation formulation.* These are given by equations involving the dependent variable $x(t)$ and its derivatives with respect to t .
- (2) *Integral equation formulations.* These are given by equations involving the dependent variable $x(t)$ and integrals of functions of $x(\tau)$, $\tau \leq t$.
- (3) *Differential difference equation formulations.* These are given by equations involving the dependent variable $x(t)$ and its lagged value $x(t - \tau)$ and their derivatives with respect to t .

Such formulations are suited for modelling systems with continuous time characterization.

2.5 Formulation B3

These formulations are similar to B1 except that there are two or more independent variables in the formulations. Since all the independent variables take on only discrete values, the dependent variables can be viewed as sequences with two or more indices – i.e. they are of the form N_{ii} or N_{ij} , etc. The formulations are given by equations involving the dependent variables for more than one value of the independent variables. Such formulations are called multi-dimensional difference equation formulations.

2.6 Formulation B4

In this formulation the dependent variables are continuous functions of two or more independent variables which take on a continuous range of values. Typically the dependent variables are of the form $u(t, x)$, $v(t, x, y)$ or $w(t, x, y, z)$. The formulations are given by equations involving the dependent variables and the partial derivatives of the dependent variables with respect to the independent variables. Such formulations are called partial differential equation formulations. These can be subdivided into various types, as will be indicated in Section 7.

3 Static Formulations

As mentioned earlier, static formulations are mathematical formulations involving either algebraic equations or function optimization. The former type is used, for example, in fitting curves or surfaces to a set of data points generated by a system, with the system characterized as a “black box”. The latter type is used mainly for optimizing system operation.

3.1 Algebraic Equation Formulations

The typical form for such a formulation is given by an equation

$$G(x, y, \theta) = 0 \quad (1)$$

where G is a vector function, x and y are vector variables and θ is a set of parameters. Often, x corresponds to input variables and y corresponds to output variables when the formulation is used to model a system characterized as a “black box”.

The equation is linear if x and y appear linearly in G , otherwise it is non-linear. The variables and/or the parameter can be either constrained or unconstrained.

3.2 Case Study A [Cont.] (Weight Lifting)

The system characterization for this problem was done in Chapter 3, Section 6.1. In this section we build a sequence of mathematical models which relate the weight lifted (L) to the body weight of the lifter (W) leading to a formula which can be used to calculate the handicapped weight lifted.

MODEL A.1

We assume that the relationship is given by

$$L = kW^\alpha \quad (2)$$

where k and α are constants. Then,

$$\log L = \log k + \alpha \log W \quad (3)$$

The handicapped lift L' is given by

$$L' = L/W^\alpha \quad (4)$$

with k and α obtained by fitting (3) to the data given.

Note that in the above model we have treated the system as a “black box”.

MODEL A.2

This model is an improvement over the earlier one in that it is based on simple

physiological arguments. As such the system is no longer treated as a "black box".

We assume that the lift is proportional to the average cross-sectional area of the lifter's muscle. Let A represent this area. This yields,

$$L = k_1 A \quad (5)$$

Let l represent a characteristic body length scale, typical body length, then

$$A = k_2 l^2 \quad (6)$$

and

$$W = k_3 l^3 \quad (7)$$

since body weight is proportional to body volume.

As a result, we have from (5)–(7)

$$L = k_1 k_2 l^2 = k_1 k_2 (W/k_3)^{2/3} = kW^{2/3} \quad (8)$$

where $k = k_1 k_2 k_3^{-2/3}$.

This is similar to Model A.1, except that $\alpha = 2/3$ and the only unknown parameter is k .

With this model the handicapped lift is given by (4) with $\alpha = 2/3$.

MODEL A.3

This model generalizes Model A.2. The lift is related to average cross-sectional area by

$$L = k_1 A^{\theta_1}, \quad 0 < \theta_1 < 1, \quad (9)$$

implying loss in efficiency for large size. Similarly,

$$A = k_2 l^{\theta_2}, \quad 0 < \theta_2 < 1 \quad (10)$$

implying variations in shape, and

$$W = W_0 + K_3 l^3 \quad (11)$$

implying that the total body weight consists of two parts, W_0 , the non-muscular weight and $W_1 (= K_3 l^3)$ the muscular weight. As a result we have from (9)–(11)

$$W = K(W - W_0)^\beta \quad (12)$$

where K , β and W_0 are three unknown parameters.

The handicapped lift is given by

$$L' = L/(W - W_0)^\beta \quad (13)$$

with the parameters obtained using the given data.

3.3 Function Optimization Formulations

The typical form for such a formulation is given by

$$\text{Maximize}_x f(x, \theta) \quad (14)$$

subject to a set of constraints of the form

$$G(x, \theta) \geq 0 \quad (15)$$

where f is a scalar function, G a vector function, x a vector variable and θ a set of parameters.

The above formulation is quite general. Any minimization problem or constraints of the form $G(x, \theta) \leq 0$ can be reformulated into a form given by (14) and (15). For example,

$$\text{Minimize}_x h(x, \theta) \quad (16)$$

is equivalent to (14) under the transformation

$$f(x, \theta) = -h(x, \theta) \quad (17)$$

A similar transformation can be performed on the constraints to get them into a form of equation (15).

Some special cases of the formulation are:

- (i) *Linear programming formulation*: x real and both f and G linear in x .
- (ii) *Non-linear programming formulation*: x real and either one or both f and G non-linear in x .
- (iii) *Integer programming formulation*: x integer.

3.4 Case Study C [Cont.] (Optimal Production)

The system characterization for this problem was done in Chapter 3, Section 6.3. We assume no carry-over from week to week; hence each week can be treated separately. We use the symbols as defined in the system characterization.

MODEL C.1

Consider butter production. We have

$$Z_1 = T_1 Y_1 \quad (18)$$

which relates the milk used for butter production and the butter produced. The cost of producing this butter is given by

$$c_1 Z_1 (= c_1 T_1 Y_1). \quad (19)$$

Since there is no carry-over, there is no sense in producing more butter than

what is demanded. This translates into

$$Z_1 = T_1 Y_1 \leq D_1. \quad (20)$$

Similarly, we have for cream

$$Z_2 = T_2 Y_2 \leq D_2 \quad (21)$$

with an associated cost

$$c_2 Z_2 = c_2 T_2 Y_2 \quad (22)$$

and for yoghurt we have

$$Z_3 = T_3 Y_3 \leq D_3 \quad (23)$$

with an associated cost

$$c_3 Z_3 = c_3 T_3 Y_3. \quad (24)$$

For the processed milk we have

$$Z_4 = T_4 Y_4 \leq D_4 \quad (25)$$

with an associated cost

$$c_4 Z_4 = c_4 T_4 Y_4. \quad (26)$$

The total cost of processing is equal to

$$\sum_{i=1}^4 c_i T_i Y_i \quad (27)$$

and the total revenue generated is given by

$$\sum_{i=1}^4 s_i Z_i = \sum_{i=1}^4 s_i T_i Y_i. \quad (28)$$

In addition we have a constraint given by

$$\sum_{i=1}^4 Y_i \leq X \quad (29)$$

and the cost of producing milk equals

$$c_0 X \quad (30)$$

As a result the total profit is given by

$$f(Y) = \sum_{i=1}^4 (s_i - c_i) T_i Y_i - c_0 X \quad (31)$$

subject to constraints given by (20), (21), (23), (25) and (29).

This is of the form given by (14) and (15) and the problem is to obtain optimal $T(\equiv Y_1 Y_2 Y_3 Y_4)$ to maximize f given by (31). Since Y_i , $1 \leq i \leq 4$ appear linearly in both f and in the various inequality constraints, the formulation used in modelling is a linear programming formulation.

If the selling price s_i is a function of Y_i ($1 \leq i \leq 4$), then f is non-linear in the variables Y_i ($1 \leq i \leq 4$). As a result the formulation used is a non-linear programming formulation.

4 Difference Equation Formulations

We start with formulations with one independent variable. The variables of the formulations are sequences of the form $Z(k)$ (or Z_k) with Z the dependent variable (either scalar or vector) and k corresponding to discrete values of the independent variable t . If the discrete values assumed by t are equi-spaced, then Z_k corresponds to $Z(t)$ with $t = \Delta k$, Δ being the interval of discretization.

A general difference equation formulation with one independent variable is given by an equation of the form

$$Z_{k+1} = g_k(Z_k, Z_{k-1}, \dots, Z_{k-n_k}; u_k, u_{k-1}, \dots, u_{k-m_k}; \theta_k), -\infty < k < \infty \quad (32)$$

where u_j , $-\infty < j < \infty$ is a known sequence. The structure of the equation is given by the function g_k ; the order by the integer $n_k + 1$ and the parameters by θ_k . In the above formulation the structure, the order and the parameters change with k .

Such a general formulation (i.e. the structure and the order varying with k) is of limited use in modelling as it is too complex. A simple formulation is one where these do not change with k , and is of the form

$$Z_{k+1} = g(Z_k, \dots, Z_{k-n}; u_k, \dots, u_{k-m}; \theta) \quad (33)$$

with the order of the equation being $(n + 1)$.

Note that, in the above formulation, there are no terms of the form Z_{k+j} or u_{k+j} , $j \geq 0$. This is important, because when the formulation becomes a model, k corresponds to time and Z_k corresponds to physical variables of the system characterization. Thus, terms such as Z_{k+j} and u_{k+j} imply that the future affects the past. This is meaningless, as it would violate the "principle of causality".

4.1 Classification of Difference Equations

If the function g is linear in Z_{k-j} ($0 \leq j \leq n$) and u_{k-j} ($0 \leq j \leq m$) then it is called a linear difference equation. If not, it is called a non-linear equation. Non-linear difference equations can be subdivided into different types - e.g. bilinear, polynomial, etc.

If the parameter θ_k does not change with k , then the equation is said to have time-invariant parameters; if not, it is said to have time-varying parameters.

4.2 Alternative Representation

The formulation given by (33) is a difference equation of order $(n + 1)$. By defining an enlarged vector Y_k as follows:

$$Y_k^T = [Z_k, Z_{k-1}, \dots, Z_{k-(n+1)}] \quad (34)$$

we can rewrite (33) as

$$Y_{k+1} = G(Y_k, U_k, \theta_k) \quad (35)$$

with

$$U_k^T = [u_k, u_{k-1}, \dots, u_{k-m}] \quad (36)$$

This process allows a difference equation of any order to be reduced to a higher dimensional difference equation of order one. This alternative representation is better suited for computer analysis.

4.3 Existence and Uniqueness of Solution

For the solution to exist (i.e. a sequence $Y_k[Z_k]$ which satisfies (35) [(33)]) the function $G[g]$ must be suitably constrained. If $G[g]$ is bounded for all bounded values of its arguments, then a solution will exist. To ensure uniqueness of the solution one needs to specify some extra conditions. If, in the case of (35), these conditions are given by Y_k being specified at some single value of k (e.g. $k = 0$), then the formulation is called an initial value formulation; if Y_k is specified by values for two or more values of k , then it is called a multi-point boundary value problem.

4.4 Multi-dimensional Difference Equations

In the case of two-dimensional difference equation formulations there are two independent variables and the dependent variables are doubly indexed sequences of the form $Z_{k,j}$. We shall assume that the first index (k) corresponds to time and that the second index (j) corresponds to a spatial coordinate when the formulation becomes a model. To ensure that the "principle of causality" is not violated, the formulation must ensure that $Z_{k+1,j}$ depends on only $Z_{m,n}$ with $m \leq k$. Note that there is no such restriction on n , and it can be either bigger than, smaller than, or equal to j . A typical first-order formulation is given by

$$Z_{k+1,j} = g(Z_{k,j}, Z_{k,j-1}, Z_{k,j+1}; u_{k,j}; \theta_{k,j}) \quad (37)$$

with $u_{k,j}$ being a specified double-indexed sequence.

To ensure the existence and uniqueness of the solution one needs to constrain the function g and specify two sets of conditions – initial conditions and boundary conditions. These conditions are similar to that for partial differential equations to be discussed in a later section, and hence omitted here.

Multi-dimensional difference equation formulations with three or four independent variables are straightforward extensions of the two-dimensional formulation.

4.5 Case Study E [Cont.] (World Population)

The system characterization for this problems was done in Chapter 3, Section 6.5. We consider the discrete time characterization with the time interval of discretization being a constant Δ . We first consider modelling the total population through a single variable, and later we consider a more refined characterization which involves spatial grouping.

MODEL E.1

Let N_i ($\equiv N(i)$) represent the total population at the end of the i th interval. If B_i and D_i are the births and deaths in the interval i , we have

$$N_i = N_{i-1} + B_i - D_i \quad (38)$$

We ignore the gestation period and assume that B_i and D_i are proportional to N_{i-1} , i.e.:

$$B_i = bN_{i-1} \quad (39)$$

and

$$D_i = dN_{i-1}.$$

As a consequence, we have:

$$N_i = \delta N_{i-1} \quad (40)$$

with

$$\delta = 1 + b - d. \quad (41)$$

Thus the model uses a first-order linear difference equation as a dummy. The initial condition is given by specifying N_i for some specific $i = i_0$.

MODEL E.2

This is an improvement over the earlier model in that it includes the gestation period. Let τ be the gestation period and we assume that $\Delta \ll \tau$. As a result we need to introduce parameter k such that

$$\Delta k \approx T. \quad (42)$$

In this model, then, equation (39) is modified thus:

$$B_i = nN_{i-1-k} \quad (43)$$

and

$$D_i = dN_{i-1}.$$

This implies that births in interval i are proportional to population in interval $(i-1-k)$. From (38) and (43) we have

$$N_i = (1-d)N_{i-1} + bN_{i-1-k} \quad (44)$$

implying that the model involves a linear difference equation of order $(k+1)$.

In this case the initial condition is specified by giving N_i over an interval $i_0 \leq i \leq i_0 + k$.

MODEL E.3

Model E.1 is based on a coarse system characterization, where the total population is characterized through one variable N_i . A more detailed or refined characterization is one where the planet earth is divided into J regions with N_{ij} representing the population in region j at the end of interval i .

If we ignore gestation and migration, then population changes in each region can be modelled separately by using equations of the form given by (40). However, the interesting case is where there is migration from one region to another.

Let f_i^{jk} represent the number of people migrating from region j to k ($j \neq k$) in the interval i . As a result, we have for region j ($1 \leq j \leq J$), the population changes given by

$$N_{ij} = \delta_j N_{i-1,j} - \sum_{\substack{k=1 \\ k \neq j}}^J f_i^{jk} + \sum_{\substack{k=1 \\ k \neq j}}^J f_i^{kj} \quad (45)$$

with

$$\delta_j = 1 + b_j - d_j \quad (46)$$

indicating different birth and death rates for each region.

Since the number of people migrating from region of j in the i th interval cannot exceed $N_{i-1,j}$ we have

$$\sum_{\substack{k=1 \\ k \neq j}}^J f_i^{jk} \leq N_{i-1,j} \quad (47)$$

Note we have assumed that, in any interval, a person can migrate only once.

The specific form of f_i^{jk} needs to be specified to complete the model. One simple form is as follows:

$$f_i^{jk} = \tau_{jk} N_{i-1,j} \quad \text{if } N_{i-1,j} > N_{i-1,k} \\ = 0 \quad (48)$$

otherwise with

$$\tau_{jk} > 0 \text{ and } \sum_{\substack{k=0 \\ k \neq j}}^J \tau_{jk} \leq 1 \quad \text{for } 1 \leq j \leq J. \quad (49)$$

This implies that people move only from more populated regions to less populated regions. We can view τ_{jk} as an indicator of the attractiveness of region k to a person living in region j .

Note that the underlying formulation of the model is a two-dimensional difference equation. The total population is obtained by summing the population over all regions. The initial conditions are specified by giving N_{ij} for $1 \leq j \leq J$, for some specific $i = i_0$.

5 Ordinary Differential Equation (O.D.E.) Formulations

A general ordinary differential equation is a mathematical formulation of the form

$$\alpha(t) D^{(n)} z(t) = g\{z(t), Dz(t), \dots, D^{(n-1)} z(t); u(t), Du(t), \dots, D^{(m-1)} u(t), \theta(t)\} \quad (50)$$

where D is the derivative operator, i.e. $Dz(t) = dz(t)/dt$ and $D^{(n)} z(t) = D(D^{(n-1)} z(t))$; $u(t)$ is a specified function which is differentiable m times; $z(t)$ is the dependent variable (either scalar or vector); $\theta(t)$ and $\alpha(t)$ are the parameters and t is the real valued independent variable. The interval of interest is given by T . Without loss of generality we assume that $0 \leq t < T$ with T being either finite or infinite.

When the formulation becomes a model, t represents time and $z(t)$ and $u(t)$ the variables of the system characterization.

5.1 Classification of O.D.E.s

The equation is said to be of order n if the highest derivative of the dependent variable is of order n .

If the parameter $\alpha(t)$, the coefficient of the highest derivative of the dependent variable, is non-zero over the interval of interest, then the equation is said to be *non-singular*; if not, it is said to be *singular*. In the case of the non-singular equation we can set the coefficient of the highest derivative to one, by dividing both sides of the equation by $\alpha(t)$.

If $u(t)$ is equal to zero over the interval of interest and $\theta(t)$ does not depend on t , then the equation is said to be *autonomous*; if not, it is called *non-autonomous*.

If the function g is linear in $z(t)$ and $y(t)$ and their derivatives, then it is called a *linear equation*; otherwise, it is called a *non-linear equation*.

If $\theta(t)$ does not change with t then the parameters of the equation are said to be *time invariant*. If not, they are said to be *time-varying*.

5.2 Alternative Representation

The formulation given in (50) is of order n . Assume that $\alpha(t) = 1$ and define an enlarged vector $y(t)$ as follows:

$$Y(t) = [z(t), Dz(t), \dots, D^{(n-1)} z(t)]^T. \quad (51)$$

Then (50) can be rewritten as

$$DY(t) = G(Y(t), U(t), \theta(t)) \quad (52)$$

where

$$U(t) = [u(t), Du(t), \dots, D^{(m-1)} u(t)]^T. \quad (53)$$

Thus the equation is reduced to a first-order differential equation with the

dependent variable $Y(t)$ being a vector of larger dimension. This representation is often better suited for both analytical and computational analysis.

5.3 Existence and Uniqueness of Solution

For the solution to exist (i.e. a function $Y(t)$ [$z(t)$] which satisfies (53) [(51)] over the interval of interest) the function $G[g]$ must be suitably constrained. To ensure that the solution is unique one needs to specify some extra conditions. In the case of (53), if these conditions are given by $Y(t)$ being specified at some single value of t (e.g. $t = 0$), then the formulation is called an initial value formulation; if $Y(t)$ is specified in terms of its values at two or more values of t , then it is called a two- or multi-point boundary value formulation.

5.4 Case Study D [Cont.] (Rocket Launch)

The system characterization for this problem was done in Chapter 3, Section 6.4. We shall assume that interaction with celestial objects other than the earth is not significant, and hence can be ignored.

MODEL D.1

Using the symbols of the system characterization and the free-body diagram shown in Figure 3.11, we have from the laws of dynamics

$$Mx''(t) = F(t) - G - f \quad (54)$$

where F is the thrust generated on the rocket; G is the gravitational force of attraction; f the frictional retarding force and M the mass of the rocket. Note that the variable $x(t)$ represents the distance of the rocket from the surface of the earth measured outwards.

From the inverse square law for gravitational attraction we have

$$G = \frac{Mg_0R^2}{(x(t) + R)^2} \quad (55)$$

where R is the radius of the earth and g_0 is the gravitational constant.

The frictional force f depends on the velocity $x'(t)$ as well as the density of air, which varies with the position $x(t)$. A general form for f is

$$f = f(x(t), x'(t)) \quad (56)$$

We assume that the density variation can be ignored, and that the frictional force varies linearly with the velocity. This results in a form

$$f = kx'(t) \quad (57)$$

where k is a constant.

If we assume that the thrust generated lasts only for a very short time we can

treat it as an impulse, resulting in

$$F(t) = F_m\delta(t) \quad (58)$$

where $\delta(t)$ is the Dirac delta function. Note we have assumed that the rocket is launched at $t = 0$ and as a consequence we have the initial conditions given by

$$x(0) = 0 \quad \text{and} \quad x'(0) = 0. \quad (59)$$

Thus the model is given by

$$Mx''(t) = F_m\delta(t) - \frac{Mg_0R^2}{(x(t) + R)^2} - kx'(t) \quad (60)$$

with the initial condition given by (59). Note that the model involves a non-linear differential equation formulation.

5.5 Case Study E [Cont.] (World Population)

The system characterization for this problem was done in Chapter 3, Section 6.5, and in Section 4.5 of this chapter we examined a few models based on discrete time characterization. In this section we discuss modelling the system with continuous time characterization.

MODEL E.4

This is the continuous time counterpart of Model E.1. Let $N(t)$ represent the total population at time t . In the interval $(t, t + \delta t)$, $N(t)$ changes due to births and deaths. As a result, we have

$$N(t + \delta t) = N(t) + aN(t)\delta t - bN(t)\delta t \quad (61)$$

where b and d are the birth and death rates, and are constant.

In going through the limit, we have

$$\lim_{\delta t \rightarrow 0} \{N(t + \delta t) - N(t)\} / \delta t = N'(t) = (b - d)N(t). \quad (62)$$

Thus the model is given by a simple first-order linear differential equation of the form

$$N'(t) = \alpha N(t) \quad (63)$$

with

$$\alpha = b - d \quad (64)$$

and the initial condition by specifying $N(t)$ at some time instant t_0 .

MODEL E.5

In the earlier model we assumed that both the birth rate and the death rate are constant. As a result α , given by (64), is a constant. A more realistic formulation

is one where α changes with $N(t)$, since there are finite limits to resources to support a population. Let the relationship between $N(t)$ and α be given by a general non-linear equation of the form

$$\alpha = f(N(t), \theta) \quad (65)$$

where θ is a set of parameters. This implies that the model is given by a non-linear differential equation

$$N'(t) = f(N(t), \theta)N(t). \quad (66)$$

Various forms for $f(N(t), \theta)$ can be used. We indicate a few:

$$(i) f(N(t), \theta) = \theta_0 \{L - N(t)\} \quad (67)$$

$$(ii) f(N(t), \theta) = \{\theta_1 - \rho \log N(t)\} \quad (68)$$

$$(iii) f(N(t), \theta) = \theta_2 \{L - N(t)\}^{1/\theta_3} \quad (69)$$

In the case of (i) and (iii) we have $N(t) \rightarrow L$ and in the case of (ii) $N(t) \rightarrow e^{\theta_1/\rho}$ as $t \rightarrow \infty$. This implies that, in these model formulations, the total population $N(t)$ is bounded. The initial condition is specified by $N(t)$ at some time instant t_0 .

MODEL E.6

We now consider modelling when the system characterization differentiates the two sexes. The variables are $N_m(t)$ and $N_f(t)$ – the total male and female population at time t . Let d_m and d_f represent the death rates for the males and the females respectively. Let $\Lambda(N_m(t), N_f(t))\delta t$ represent births taking place in $(t, t + \delta t)$ if there be $N_m(t)$ males and $N_f(t)$ females at time t , and let α represent the fraction of male births. Then, using an argument similar to that in Model E.4, we have

$$N'_m(t) = -d_m N_m(t) + \alpha \Lambda(N_m(t), N_f(t)) \quad (70)$$

$$N'_f(t) = -d_f N_f(t) + (1 - \alpha) \Lambda(N_m(t), N_f(t))$$

and the total population at time t given by

$$N(t) = N_m(t) + N_f(t). \quad (71)$$

If $\alpha = 0.5$, then half the new births are males.

One needs to specify the form of $\Lambda(N_m(t), N_f(t))$ to complete the model. Two forms are as follows:

$$(i) \Lambda(N_m(t), N_f(t)) = \lambda_1 \min \{N_m(t), N_f(t)\}, \text{ and} \quad (72)$$

$$(ii) \Lambda(N_m(t), N_f(t)) = \lambda_2 \sqrt{N_m(t)N_f(t)}. \quad (73)$$

λ_1 and λ_2 being constants. In either case the resulting formulation is given by a pair of coupled non-linear ordinary differential equations.

The initial conditions are given by $N_m(t)$ and $N_f(t)$ for some specified value t_0 .

6 Differential Difference Equation (D.D.E.) Formulations

A fairly general first-order differential difference equation formulation, with one dependent variable, is given by

$$z'(t) = f(z(t), z(t - \tau_1), z(t - \tau_2), \dots, z(t - \tau_p); u(t)). \quad (74)$$

The parameters $\tau_1, \tau_2, \dots, \tau_p$ can be either functions of t (the independent variable) or constants. $u(t)$ is a known function. $\tau_i \geq 0$ ($1 \leq i \leq p$), in order to ensure that the “principle of causality” is not violated when the formulation becomes a model.

Higher order D.D.E. involve higher derivatives of z , and using the technique of Section 5.2 one can reduce it to a vector first-order D.D.E. With two or more dependent variables the formulation is similar to (74) comprising a set of coupled equations. We shall omit the classification as it is similar to that for the ordinary differential equations (see Section 5.1).

To ensure that a solution exists the function f must be constrained, and to ensure that the solution is unique one needs to specify $z(t)$ over a non-zero interval of t which is longer than the largest value of τ_i , $1 \leq i \leq p$. This is in contrast to the ordinary differential equation formulation, where for a first-order equation one needs to specify the dependent variable for a specific point t_0 .

6.1 Case Study E [Cont.] (World Population)

MODEL E.7

Consider the continuous time system characterization for the problem discussed in Chapter 3, Section 6.5. We are interested in the total population $N(t)$. This changes due to births and deaths. If we include the gestation period, then the population change in the interval $(t, t + \delta t)$ is given by

$$N(t + \delta t) - N(t) = \{bN(t - \tau) - dN(t)\}\delta t \quad (75)$$

where b and d are the birth and death rates and τ is the gestation period. This follows as births in the interval $(t, t + \delta t)$ depend on the population at $(t - \tau)$. Going through the limiting process, we have the model given by

$$N'(t) = bN(t - \tau) - dN(t), \quad (76)$$

involving a D.D.E. formulation of order 1. The initial condition is given by $N(t)$, $-\tau \leq t \leq 0$, so that the model can be used to obtain $N(t)$ for $t > 0$.

7 Partial Differential Equation (P.D.E.) Formulations

Partial differential equation formulations involve the partial derivatives of one or more dependent variables, each of which is a function of two or more independent variables. We first discuss formulation involving two independent variables.

7.1 Formulations with Two Independent Variables

Let x and t represent the two independent variables, and the dependent variables are functions of the form $u(x, t)$. Let partial derivatives be denoted by $u_t, u_x, u_{tt}, u_{xx}, u_{tx}$, etc., where $u_t = \partial u / \partial t$, $u_x = \partial u / \partial x$ and so on.

A general P.D.E. with one dependent variable is given by

$$g(u, u_x, u_t, u_{xx}, u_{xt}, u_{tt}, \dots, \theta(x, t), f(x, t)) = 0 \quad (77)$$

where $\theta(x, t)$ is a set of parameters and $f(x, t)$ is a known function. The order of the P.D.E. is given by the highest partial derivative occurring in the formulation.

As a part of the formulation one needs to define the domain of the independent variables x and t . It could take various forms, e.g.:

- (i) $t \geq 0, L_1 \leq x \leq L_2$, or
- (ii) $t \geq 0, L_1 \leq x < \infty$, or
- (iii) $t \geq 0, -\infty < x < \infty$

where L_1 and L_2 are finite.

When such formulations model a system, t corresponds to time; x corresponds to a spatial coordinate and $u(x, t)$ corresponds to a variable of the system characterization.

7.2 Classification of P.D.E.

If the dependent variable $u(x, t)$ and its partial derivative appear linearly in g then the equation is said to be *linear*. If not, it is called a *non-linear* equation.

A fairly general, second-order linear P.D.E. is given by:

$$au_{tt} + 2bu_{tx} + cu_{xx} + du_t + eu_x + gu = f(x, t) \quad (78)$$

where the parameters a, b, c, d, e and g are either constants or functions of the independent variables x and t . This equation can be subdivided into three types based on the sign of Γ , given by

$$\Gamma \equiv \Gamma(x, t) = b^2(x, t) - a(x, t)c(x, t) \quad (79)$$

At a point (x, t) in the domain of the independent variables, the equation is called:

- (i) *parabolic* if $\Gamma = 0$,

- (ii) *hyperbolic* if $\Gamma > 0$, and
- (iii) *elliptic* if $\Gamma < 0$.

If the parameters a, b and c are constants then the equation is either parabolic or hyperbolic or elliptic over the whole domain of the independent variables.

7.3 Existence and Uniqueness of Solution

For the solution to exist, the function g must be suitably constrained. To ensure uniqueness one needs to specify additional conditions.

The number of conditions needed depends on the order of the differential equation and the nature of the conditions depend on the range of the independent variables.

In the case of a first-order P.D.E., one could specify the condition by specifying $u(x, t)$ along a curve in the $x-t$ plane. If it is of the form

$$u(x, 0) = r(x) \quad (80)$$

where $r(x)$ is a known function, then the formulation is called an initial value formulation.

For a second-order parabolic equation a set of conditions which will ensure uniqueness is given by one initial condition (I.C.) and two boundary conditions (B.C.). For example, if $0 \leq t < \infty$ and $-\infty < x < \infty$, the following conditions

$$\text{I.C.: } u(x, 0) = f_0(x); \quad -\infty < x < \infty \quad (81)$$

$$\text{B.C.: } |u(x, t)| < \infty \text{ as } x \rightarrow \pm \infty$$

are sufficient to ensure that the solution is unique.

For a second-order hyperbolic equation a set of conditions which will ensure uniqueness is given by two initial conditions (I.C.) and two boundary conditions (B.C.). For example, if $0 \leq t < \infty$ and $L_1 \leq x \leq L_2$, then the following conditions:

$$\text{I.C.: } \begin{cases} u(x, 0) = f_0(x) \\ \partial u(x, 0) / \partial t = f_1(x) \end{cases} \quad L_1 \leq x \leq L_2 \quad (82)$$

$$\text{B.C.: } \begin{cases} u(L_1, t) = g_1(t) \\ u(L_2, t) = g_2(t) \end{cases} \quad 0 \leq t < \infty \quad (83)$$

are sufficient to ensure that the solution is unique.

7.4 Case Study E [Cont.] (World Population)

In Sections 4.5 and 5.5 we examined several models based on different system characterizations. In this section we discuss modelling population changes with a system characterization which takes into account the age structure of

the population and treats time as being continuous. This leads to a P.D.E. formulation.

MODEL E.8

Let $N(t, x)$ be a variable characterizing the age structure of the population at time t . More specifically, the population in the age group l_1 to l_2 is given by

$$\int_{l_1}^{l_2} N(t, x) dx \quad (84)$$

The birth and death rates are given by functions $b(x)$ and $d(x)$ and are of the form as shown in Figure 3.14 and described in Section 6.5 of Chapter 3. The range for the independent variables are $0 \leq t < \infty$ and $0 \leq x \leq x_m$ where x_m is the upper limit to human age.

If we consider a small age interval – e.g. $(x, x + \delta x)$, then the total population in this age group at time t is given by

$$N(x, t)\delta x + O(\delta x^2) \quad (85)$$

Thus,

$$N(x, t + \delta t)\delta x = N(x - \delta t, t)\delta x - N(x - \delta t, t)d(x)\delta x + O(\delta x^2). \quad (86)$$

The first term represents people in the age group $(x - \delta t, x)$ at time t and the second term represents the reduction due to deaths.

On expanding using Taylor series and taking the limit, we have

$$\frac{\partial N(x, t)}{\partial t} = -\frac{\partial N(x, t)}{\partial x} - d(x)N(x, t)$$

or

$$\frac{\partial N(x, t)}{\partial t} + \frac{\partial N(x, t)}{\partial x} = -d(x)N(x, t) \quad (87)$$

New additions at time t are given by

$$N(0, t) = \int_0^{x_m} b(x)N(x, t)dx \quad (88)$$

Note that in deriving the above equation we have ignored the gestation period.

Equation (88) can be viewed as a boundary condition. Since $d(x) \rightarrow \infty$ as $x \rightarrow x_m$ (to ensure that no-one survives beyond x_m) we have $N(x_m, t) = 0$. The initial condition is given by specifying $N(x, t)$ for some t_0 – viz.

$$N(x, t_0) = G(x), \quad 0 \leq x \leq x_m \quad (89)$$

Thus, in this case, the model involves a linear first-order partial differential equation formulation as a dummy.

7.5 Case Study F [Cont.] (River Pollution)

The system characterization for this problem was done in Chapter 3, Section 6.6. In this section we discuss building of a model using the simplest characterization where the river is viewed as a one-dimensional channel with constant cross-section.

MODEL F.1

Let $T(x, t)$ represent the concentration level of pollution at a distance x from the point of discharge at time t . From the system characterization we have

$$-L_1 \leq x \leq L_2 \quad \text{and} \quad 0 \leq t < \infty \quad (90)$$

which define the range of the independent variables.

The concentration level changes due to diffusion and transportation. Let D be the coefficient of diffusion and let U be the velocity of the river which is assumed to be constant. The diffusion is governed by Fick's first law of diffusion, which states that the diffusion current vector J is given by

$$J = -D \partial T(x, t) / \partial x \quad (91)$$

From the equation of continuity for the diffusing substance, we have

$$\frac{\partial T(x, t)}{\partial t} = -U \frac{\partial T(x, t)}{\partial x} + D \frac{\partial^2 T(x, t)}{\partial x^2} \quad (92)$$

This is obtained by considering a small volume centred at x at time t and evaluating the net inflow and outflow of pollution in a small time δt . The net change in the small volume can be related to the net inflow and outflow and in the limit $\delta t \rightarrow 0$ and $\delta x \rightarrow 0$ we have the above equation.

Thus, from (78) and (79) we see that the model involves a parabolic partial differential equation. We need to specify additional conditions to ensure uniqueness of the solution. These are given by

$$\text{I.C.: } T(x, 0) = G(x), \quad -L_1 \leq x \leq L_2 \quad (93)$$

indicating the concentration levels along the river at $t = 0$, and

$$\begin{aligned} \text{B.C.: } T(-L_1, t) &= 0 \\ T(L_2, t) &= 0 \quad 0 < t < \infty \end{aligned} \quad (94)$$

The above model does not take into account the discharge of pollution at $x = 0$. This can be easily accounted for by modifying (92) to include an extra term $F(x, t)$ which is of the form

$$F(x, t) = \alpha g(t) \delta(x) \quad (95)$$

where $g(t)$ is the time history of dumping and $\delta(x)$ is the Dirac delta function.

7.6 P.D.E. Formulations with More than Two Independent Variables

The dependent variables are functions of three or four independent variables and are of the form $u(x, y, t)$ or $u(x, y, z, t)$. A general differential equation is of the form given by (77) but involving partial derivatives with respect to all the independent variables – i.e. the formulations are straightforward extensions of the two independent variable case.

Notes and References

Function optimization formulations belong to the theory of mathematical programming. Items [1] and [2] give a small sample of books on this topic. Dynamic optimization formulations have also been studied extensively and [3] is an introductory text on the subject. Items [4]–[10] are an illustrative sample of books on the application of optimization models in different disciplines.

Difference equation formulations have received less attention relative to differential equation formulations. For more on difference equations see [11]–[13]. The last reference deals with the use of difference equation formulations in modelling physical systems.

The large number of books on ordinary differential equations can be broadly divided into two categories. Those belonging to the first category concentrate on theoretical aspects (for example, existence and uniqueness of solutions) and vary from introductory to advanced (e.g. [14] and [15]). Books belonging to the second category (e.g. [16]–[20]) concentrate on the methods of solution and their applications. Item [21] is an interesting book which not only deals with applications but also contains interesting historical notes. Items [22]–[24] are four introductory-level books which deal with low-order differential equation formulations and their use as models for solving a diverse range of problems.

For more on differential difference equations see [25]–[27]. Such formulations have been used extensively in modelling biological systems (e.g. [28]). We have not discussed integral and integro-differential equation formulations; [29]–[31] give a small sample of books on this topic.

There are many books which discuss partial differential equations. As with books on ordinary differential equations, some concentrate on theoretical aspects, whilst others deal with techniques of analysis and applications. Items [32]–[38] are a small sample of books belonging to the second category. In addition, there are advanced-level books dealing with specific formulations – for example, [39] deals with parabolic equation formulations and [40] and [41] deal with hyperbolic equation formulations.

We have not discussed a particular class of mathematical formulations belonging to catastrophe theory. These formulations have been successfully

used to model the qualitative behaviour of a wide range of systems and phenomena. For an introductory presentation see [42] and for more details see [43]–[45].

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CHAPTER 6

Analysis of Mathematical Formulations – I

1 Introduction

Once a mathematical model is constructed (by associating an abstract mathematical formulation with the variables of the system characterization) the next step is to obtain the behaviour of the model. This is done by the following three-step procedure.

- Step 1:* Discard the association (mentioned above) so that only the mathematical formulation is retained.
- Step 2:* Carry out an analysis of the formulation using appropriate mathematical techniques.
- Step 3:* Re-introduce the discarded association so that the analysis can be interpreted in terms of the physical variables of the system characterization to yield model behaviour.

In this chapter we focus our attention on the analysis of mathematical formulations considered in the previous chapter. As such, we start with a brief discussion on the different types of analysis.

2 Types of Analysis

Broadly speaking, the analysis of mathematical formulations can be either qualitative or quantitative. As the name suggests, *qualitative analysis* deals with the study of qualitative aspects of a given mathematical formulation without explicitly solving it. This is done by an analysis of the underlying mathematical structure of the formulation. Typically, such an analysis provides answers to questions of the form:

- (a) Is the solution of a given O.D.E. formulation periodic?

- (b) Does the solution of a given difference equation formulation go to zero as the index n approaches infinity?

The answer is usually binary valued, i.e. of the form yes or no.

In contrast, *quantitative analysis* is concerned with finding the explicit solution which satisfies the given mathematical formulation. Quantitative analysis can be divided into two types, as indicated below: analytical methods and computational methods. Both these play an important role in mathematical modelling. Each of these can be further subdivided as indicated below.

2.1 Analytical Method of Analysis

In this method the solution to a given mathematical formulation is obtained in terms of an analytical expression involving the parameters and the independent variables of the formulation. The solution can be either exact or approximate, depending on whether the solution satisfies the formulation (i.e. the equations and the associated conditions) exactly or approximately.

Only for a small class of mathematical formulations is it possible to obtain exact analytical solutions. Approximate solutions are sought when it is either extremely difficult, or impossible, to obtain an exact solution. The approximate solution is often obtained as an exact solution of a modified mathematical formulation which is close to the original formulation in some sense.

2.2 Computational Method of Analysis

In this method the solution is obtained using a computer. The solution is only approximate and depends on the type of computer and the method used.

Analytical methods of analysis yield parameterized solutions – that is, the solutions are analytical expressions of the parameters of the mathematical formulations. In contrast, computational methods of analysis yield solutions for specific numerical values of the parameters. Hence, in the latter case, the solutions have to be recomputed every time the parameter values are altered.

Another difference is that analytical methods of analysis are applicable only to a small class of mathematical formulations. They are of limited use in determining model behaviour of complex systems. In contrast, computational methods of analysis are applicable to a much wider class of mathematical formulations.

3 Types of Computers and the Nature of Computed Solutions

In this section we first discuss the different types of computers available for solving mathematical formulations, the different approaches to computation they require and the nature of the computed solutions. There are essentially

three types of computers – digital, analog and hybrid. The essential features of each will be discussed in turn.

3.1 The Digital Computer and Digital Computing

A digital computer operates with real and integer numbers stored as binary digits. As a consequence the computer stores real variables only approximately, because of the limited precision due to finite word length and continuous functions as sequences for discrete values of the argument. The operations are executed according to a pre-specified program – a set of instructions which the computer recognizes and executes sequentially.

In general, the program is written in a higher-level language and the computer translates this into a binary pattern before it can execute it. For solving specific mathematical formulations (e.g. O.D.E. formulations) one can either use a general higher-level language (e.g. Fortran, Pascal) or a special higher-level language especially designed for solving specific formulations (e.g. CSMP for O.D.E. formulations). The former offers greater flexibility at the expense of greater programming effort from the user, while the latter requires less programming but is also less flexible. Some specific higher-level languages (also called simulation languages) will be discussed in Chapter 9.

Because of the nature of the computer, *the solutions of dynamic formulations with continuous independent variables can in general be obtained only for discrete values of the independent variables*. We should mention, however, that there exist very high-level languages and programs (for example, MACSYMA) which can perform symbolic manipulations on the continuous variables. The study of different methods for solving mathematical formulations on digital computers belong to the theory of “numerical methods”. We shall discuss some specific methods for solving different formulations later in the chapter.

3.2 The Analog Computer and Analog Computing

Analog computers operate with variables represented as electrical voltages. The computer consists of a variety of blocks or components satisfying different mathematical relationships between the input and the output voltages – e.g. integration, addition to name only two. By linking the components physically (also called patching) the voltages of different components become related and satisfy the desired mathematical formulation. The solution is thus given either by the voltage, or time history of the voltage, of one or more components. *The analog computer is ideally suited to solving dynamic formulations with one independent variable*. The independent variable is represented as a continuous variable on the computer. When the formulation contains two or more independent continuous variables, only one of them can be represented continuously on the computer. In this case the solutions are obtained as a (continuous) function of one independent variable for discrete values of the

remaining independent variables. Since the range of electrical voltages is finite, the formulation needs to be scaled so that the electrical voltages representing different variables do not exceed the machine limits. The process of scaling is similar to dimensional analysis – a topic to be discussed in the next section. We should mention that while analog computers “went out of fashion” during the past two decades, there seems to be a resurgence of interest in them in the field of neural network computing systems, where they are used as components of an essentially digital system.

3.3 The Hybrid Computer and Hybrid Computing

The hybrid computer is an analog computer connected to a digital computer. The advantage of such a configuration is that it combines the best features of both machines, and at the same time allows the programmer to overcome the worst features of either. Since the mode of operation of each machine is different (viz. digital vs analog, discrete vs continuous and series vs parallel) a proper interface is needed to establish effective communication between the two machines.

3.4 Changing Emphasis in Computing

With the developments in digital computers over the past ten years, and the availability of a large number of computer packages for solving different mathematical formulations, the use of analog and hybrid computers is becoming less popular except for the neural aspects mentioned above, which are still at the research stage. Hence, in the remainder of this chapter we shall confine our discussion of computational methods to those used in digital computing. In Chapter 9 we will return to the use of analog computers in solving different mathematical formulations.

4 Dimensional Analysis and Scaling

Since a mathematical model represents a real physical system, often the variables and parameters of the model can be viewed as having physical dimensions and are characterized through basic fundamental units such as mass (M), length (L) and time (T). This point of view is useful for, through it, the consistency of a model can be checked to ensure that it is in agreement with the physical aspects of the system. Our interest in this section is to use this information for dimensional grouping and scaling.

4.1 Dimensional Grouping

Instead of dealing with the original variables and parameters of a given formulation, it is often desirable to consider groupings of variables and parameters. As a result the original set of variables and parameters are

replaced by a new set, and the formulation restated in terms of this new set. By proper grouping the new set can be made non-dimensional, and if some of the new parameters can be identified as being small they can be ignored in certain instances. The advantage of this is that the resulting formulation may be simpler and hence easier to solve. Great care must be taken in this simplification process or else the solution of the simplified formulation might bear very little resemblance to the true solution of the original formulation. Successful dimensional analysis and simplification requires a deep understanding of time and length scales associated with the variables of the system being modelled, and a well-developed intuition. This is illustrated in the following case study.

4.2 Case Study D [Cont.] (Rocket Launch)

In Section 5.4 of Chapter 5 we discussed the mathematical modelling of this problem. If the frictional force can be ignored and the thrust can be treated as an impulse, the model is given by

$$Mx''(t) = F_m \delta(t) - Mg_0 R^2 / (R + x(t))^2 \quad (1)$$

where the primes denote derivatives. The initial conditions are given by

$$x(0) = 0 \quad \text{and} \quad x'(0) = 0 \quad (2)$$

Because the thrust acts as an impulse, (1) and (2) can be rewritten as

$$x''(t) = -g_0 R^2 / (R + x(t))^2 \quad (3)$$

with

$$x(0) = 0 \quad \text{and} \quad x'(0) = V = F_m / M \quad (4)$$

Let us assume that $x(t) \ll R$. In this case we can simplify the equation to

$$x''(t) = -g_0 \quad (5)$$

By this simplification we have converted the non-linear equation (3) into the linear equation (5). However, we cannot be sure if the assumption $x(t) \ll R$ is valid. This would depend on the value of V , and it is not obvious as to what the relationship between V , g and R is to ensure that the simplification is valid.

Towards this end, we use dimensional analysis to define non-dimensional groupings of variables to test the validity of our assumption. The dimensions of the various variables and parameters in the original formulation are as follows:

		Dimension
Dependent variable	x	L
Independent variable	t	T
Parameter	g_0	LT^{-2}
Parameter	V	LT^{-1}
Parameter	R	L

Let τ and $y(\tau)$ be the new set of variables obtained by the non-dimensional grouping of the original variables. We consider three different selections of groupings.

Grouping 1: Let $\tau = t/RV^{-1}$ and $y(\tau) = x(t)/R$. Then (3) can be written as

$$\varepsilon \frac{d^2 y(\tau)}{d\tau^2} = -\frac{1}{(y(\tau) + 1)^2}, \quad y(0) = 0, \quad \dot{y}(0) = 1 \quad (6)$$

with

$$\varepsilon = V^2/g_0 R \quad (7)$$

Grouping 2: Let $\tau = t/\sqrt{Rg_0^{-1}}$ and $y(\tau) = x(t)/R$. Then (3) can be rewritten as

$$\frac{d^2 y(\tau)}{d\tau^2} = -\frac{1}{(y(\tau) + 1)^2}, \quad y(0) = 0, \quad \dot{y}(0) = \varepsilon \quad (8)$$

with ε as defined above.

Grouping 3: Let $\tau = t/Vg_0^{-1}$ and $y(\tau) = x(t)/V^2g_0^{-1}$. Then (3) can be rewritten as

$$\frac{d^2 y(\tau)}{d\tau^2} = -\frac{1}{(1 + \varepsilon y(\tau))^2}, \quad y(0) = 0, \quad \dot{y}(0) = 1 \quad (9)$$

with ε as defined above.

If $V^2 \ll g_0 R$, then $\varepsilon \ll 1$. In this case we can ignore ε and obtain an approximate solution. The groupings 1 and 2 are not useful. With these the solutions obtained by setting ε to zero bear no relation to the original solution. However, grouping 3 yields a solution which is fairly close to that of the original formulation when ε is set to zero. Furthermore, it leads to a linear equation (as opposed to the original equation which is non-linear) and therefore much easier to solve.

4.3 Scaling

Scaling amounts to non-dimensionalizing, so that the relative magnitude of each term is indicated by a factor preceding the term. More formally, in the process of scaling one attempts to select intrinsic reference quantities so that each term in the dimensional equation can be written as a factor (which closely estimates the term's order of magnitude) and a dimensionless factor of unit magnitude. Thus if $x(t)$ be a variable of the formulation and x_m the absolute maximum value of it, then it is replaced by $x_m y(t)$ with $y(t) = x(t)/x_m$ resulting in a dimensionless variable $y(t)$ of magnitude less than or equal to unity. The selection of suitable intrinsic reference quantities is closely related to length and time scales of the system. We illustrate this by again considering the rocket launch problem.

4.4 Case Study D [Cont.]: (Rocket Launch)

Since we start with the assumption that $x \ll R$, we have the rocket move with a deceleration proportional to g starting with an initial velocity V . As a result the rocket velocity decreases and reaches zero value at $x = x_m$, the maximum height reached by the rocket. The time taken to reach this height is V/g_0 and the mean velocity during this period can be taken to be $V/2$. Thus the maximum altitude reached by the rocket is roughly $V^2/2g_0$. In other words, x_m is of the order V^2/g_0 . (Note: If we include the factor $1/2$, we would get a more accurate estimate.) This suggests an intrinsic length scale of V^2/g_0 . Similarly, an intrinsic time scale is V/g_0 . Using these intrinsic length and time scales, we can scale the variables as follows:

$$\tau = t/Vg_0^{-1} \text{ and } y(\tau) = x(t)/V^2g_0^{-1} \quad (10)$$

This is precisely the combination for grouping 3 of Section 4.2, which led to approximate solutions which are close to the true solution.

5 Static Formulations

In Section 3 of Chapter 5 we discussed two types of static formulations - algebraic equation and function optimization formulations. In this section we briefly discuss some aspects of the analysis of such formulations.

5.1 Algebraic Equation Formulations

A general formulation is given by a multi-dimensional function

$$G(x, y, \theta) = 0 \quad (11)$$

x and y being vector variables and θ being a vector parameter. A typical problem in analysis is the following. Given x and θ find y which satisfies (11). (This corresponds to finding the model output given the input and model parameters.) The solution y might not exist. If it does, it might or might not be unique.

5.1.1 ANALYTICAL SOLUTIONS

Only for a small class of formulations is it possible to obtain y analytically as a function of x and θ . One such is when (11) has the form

$$A(x, \theta)y + B(x, \theta) = 0 \quad (12)$$

and $A(x, \theta)$ is a non-singular $n \times n$ matrix. In this case a unique solution exists and is obtained by inverting the matrix $A(x, \theta)$. In the above formulation y is a $n \times 1$ vector which appears linearly in the equation. When y appears non-linearly, then there can be multiple solutions and one would need a computational scheme to obtain them.

5.1.2 COMPUTATIONAL SOLUTIONS

We shall suppress writing x and θ for notational convenience. Hence (11) will be written as $G(y) = 0$. Let y and $G(y)$ be n -dimensional vectors. Define

$$g(y) = y - A(y)G(y) \quad (13)$$

with $A(y)$ being a non-singular $n \times n$ matrix. Consider the equation

$$y = g(y) \quad (14)$$

It is easily seen that (11) and (14) have the same set of solutions. The solutions for (14) can be obtained by the following iteration scheme:

$$y_{k+1} = g(y_k), \quad k = 0, 1, 2, \dots \quad (15)$$

with y_0 an arbitrary initial starting vector. The iteration will converge provided the function $g(y)$ and the initial vector y_0 satisfy some conditions.

The simplest choice is $A(y) = A$ a constant matrix. An alternative is $A(y) = J^{-1}(y)$, where $J(y)$ is the Jacobian matrix (i.e. $J(y) = \partial G(y)/\partial y$), provided the inverse exists. The latter has a faster rate of convergence but is achieved at the expense of extra computation (i.e. evaluation and inversion of the Jacobian matrix) at each step of the iteration. Other schemes are obtained by different choices for $A(y)$.

5.1.3 REFORMULATION OF THE PROBLEM

The solution to (11) can be obtained by reformulating the problem as a function minimization problem. Consider the problem of finding y to minimize $H(y)$ given by

$$H(y) = G^T(y)G(y) = \sum_{i=1}^n \{G_i(y)\}^2 \quad (16)$$

where $G_i(y)$, $1 \leq i \leq n$, are the components of $G(y)$. Since $H(y) \geq 0$, the optimal y which minimizes $H(y)$ is the one which results in $H(y)$ being zero. This optimal y also satisfies (11). The minimization problem will be discussed in the next subsection.

5.2 Function Optimization Formulations

A typical formulation is as follows. Find an n -dimensional vector x which minimizes a scalar function $f(x)$ (often called the objective function). (Note: For notational convenience we omit the parameters of the functions, i.e. we write $f(x)$ instead of $f(x, \theta)$, and so on.) We assume that x is a real variable. The case where x is either an integer, or part integer and part real variable, needs to be treated differently. When x is unconstrained then we have an unconstrained optimization problem. When x is constrained to satisfy a constraint of the

form

$$G(x) \leq 0 \quad \text{or} \quad G(x) = 0 \quad (17)$$

we have a constrained optimization problem. If the constraint involves strict equality, then it is called an equality constraint; otherwise it is called an inequality constraint. As indicated in Chapter 5, formulation involving maximization instead of minimization, or a constraint $G(x) \geq 0$, can be recast into a form involving minimization and a constraint of the form given by (17).

5.2.1 UNCONSTRAINED OPTIMIZATION

The optimal x^* which minimizes $f(x)$ must satisfy the following necessary condition

$$J(x) = \partial f(x)/\partial x = 0 \quad (18)$$

provided the derivative exists. In this case, one way of obtaining the optimal x^* is to solve (18) using the methods discussed in Section 5.1. An alternative approach is to use computational methods to minimize $f(x)$ directly.

5.2.2 COMPUTATIONAL METHODS

Since $J(x)$ given by (18) is the gradient vector, a computational method (called "gradient method") for finding the optimal x^* is the following iterative scheme:

$$x_{k+1} = x_k - t_k J(x_k), \quad k = 0, 1, \dots \quad (19)$$

where t_k is a positive scalar quantity and x_0 is chosen arbitrarily. t_k can be either constant or vary with x_k . If t_k is chosen to minimize

$$f(x_k - tJ(x_k)) \quad (20)$$

($t > 0$)

then the method involves a one-dimensional minimization at each step of the iteration. This approach is also the basis for a large number of methods. The two best known are the conjugate gradient method and the variable metric method. Under appropriate conditions x_k will converge to the optimal x^* as $k \rightarrow \infty$.

5.2.3 CONSTRAINED OPTIMIZATION

The problem is to obtain the optimal x^* which minimizes $f(x)$ subject to the constraint given by (17). One approach is to convert the constrained optimization problem into an unconstrained optimization problem and use the methods described earlier. The penalty function method is one such. An alternative approach is via Lagrange multipliers where the constraints are adjoined to $f(x)$.

5.2.4 PENALTY FUNCTION METHOD

In the penalty function method we minimize a function $F(x, k)$ given by

$$F(x, k) = f(x) + k \sum_{i=1}^m \{ \max(G_i(x), 0) \}^2 \quad (21)$$

where k is a scalar > 0 and $G_i(x)$ are the components of $G(x)$, i.e.

$$G^T(x) = [G_1(x), G_2(x), \dots, G_m(x)] \quad (22)$$

For a given k , the optimal x^* obtained by minimizing $F(x, k)$, subject to no constraint, is a function of k if one or more of the $G_i(x)$ is > 0 . This corresponds to the constraint being violated. In this case the second term is greater than zero and reflects the penalty paid for violating the constraint. As k is increased the penalty increases. This forces the optimal solution to satisfy the constraint as k approaches ∞ in the limit. In other words, the optimal solution to the constrained formulation is obtained as a limit of a sequence of optimal solutions for the unconstrained formulation.

5.2.5 LAGRANGE MULTIPLIER METHOD

We shall first consider the case of an equality constraint (i.e. $G(x) = 0$). In the method of Lagrangian multipliers the constraint is adjoined to the objective function by means of an m -dimensional Lagrangian multiplier λ ($\lambda^T = [\lambda_1, \lambda_2, \dots, \lambda_m]$) to define a function $F(x, \lambda)$ given by

$$F(x, \lambda) = f(x) + \sum_{i=1}^m \lambda_i G_i(x) \quad (23)$$

$F(x, \lambda)$ is a function of $n + m$ variables. The unconstrained minimization of this function yields an optimal x^* and λ^* . This x^* is also the optimal value of x which minimizes $f(x)$ subject to the equality constraint $G(x) = 0$. The x^* and λ^* satisfy the necessary conditions (for optimality) given by

$$\partial f(x)/\partial x + \sum_{i=1}^m \lambda_i \partial G_i(x)/\partial x = 0 \quad (24)$$

$$G(x) = 0 \quad (25)$$

For the case of optimization subject to an inequality constraint, the Lagrangian multiplier method requires that the multipliers be non-negative. The optimal x^* and λ^* which minimize $F(x, \lambda)$ satisfy the necessary conditions (for optimality) given by

$$\partial f(x)/\partial x + \sum_{i=1}^m \lambda_i \partial G_i(x)/\partial x = 0 \quad (26)$$

$$\sum_{i=1}^m \lambda_i g_i(x) = 0 \quad \lambda_i \geq 0, \quad 1 \leq i \leq m \quad (27)$$

This optimal x^* also minimizes $f(x)$ subject to the inequality constraint $G(x) \leq 0$. The method works only when the Lagrangian multipliers exist. Their existence can be assured if the constraints satisfy certain conditions. The "Kuhn-Tucker" condition is one such.

5.2.6 COMPUTATIONAL METHODS

In general, one needs a computational scheme to solve constrained formulations. A number of methods have been developed. They are all iterative in nature. Some are designed for specific forms of $f(x)$ and $G(x)$. One such is the well-known simplex method for solving linear programming formulations – formulations where both $f(x)$ and $G(x)$ are linear in x . In a linear programming formulation the admissible region for x is a convex polyhedron and the optimal x belong to the set of vertices of the convex polyhedron. The simplex method is an iterative method which moves from one vertex to another to finally converge on the vertex which yields the optimal solution.

5.3 Case Study C [Cont.] (Optimal Production)

In Section 3.4 of Chapter 5 we formulated a model (Model C1) for this problem. Using the notation of Section 3.4 of Chapter 5 and defining

$$Y^T = [Y_1, Y_2, Y_3, Y_4] \quad (28)$$

$$l^T = [(s_1 - c_1), (s_2 - c_2), (s_3 - c_3), (s_4 - c_4)] \quad (29)$$

$$b^T = [D_1, D_2, D_3, D_4, X] \quad (30)$$

$$A = \begin{bmatrix} T_1 & 0 & 0 & 0 \\ 0 & T_2 & 0 & 0 \\ 0 & 0 & T_3 & 0 \\ 0 & 0 & 0 & T_4 \\ 1 & 1 & 1 & 1 \end{bmatrix} \quad (31)$$

the model can be written as

$$\max_Y = l^T Y - c_0 X \quad (32)$$

subject to

$$AY \leq b \quad Y \geq 0. \quad (33)$$

This is a standard linear programming formulation and can be solved by the simplex method.

A large number of computer packages are available for solving linear programming formulations. They require the user to specify the entries for A , l and b . The packages contain subroutines for printing the optimal solution if it exists, and error messages if not.

6 Difference Equation Formulations

This class of formulations was discussed in Section 4 of Chapter 5. A general n th-order difference equation formulation with one independent variable is of the form

$$z_{k+1} = g(z_k, z_{k-1}, \dots, z_{k-n}; u_k, \dots, u_{k-m}; \theta_k) \quad (34)$$

with the initial condition given by an n -dimensional vector

$$(z_0, z_1, \dots, z_n) \quad (35)$$

6.1 Analytical Methods

It is possible to obtain the solution analytically only for a small class of formulation. One such is when the equation is linear and the parameters time-invariant.

6.2 Case Study E [Cont.] (World Population)

In Section 4.5 of Chapter 5 we formulated three models (Models E.1 to E.3) involving difference equation formulations.

MODEL E.1

The model is given by

$$N_i = \delta N_{i-1}, \quad i \geq 1 \quad (36)$$

with

$$\delta = 1 + b - d \quad (37)$$

Note that N_i represents the total population and b and d the birth and death rates. This is a first-order difference equation and can be solved uniquely if the initial condition N_0 is specified.

If b and d are constants, the solution can be obtained analytically and is given by

$$N_i = \delta^i N_0 \quad (38)$$

Depending on δ , the solution N_i either increases or decreases continuously with i , or else does not change at all.

If the birth rate depends on the population, δ is a function of N_{i-1} . In this case the equation is non-linear and the ability to obtain an analytic solution depends on the nature of the non-linearity.

MODEL E.3

The model is given by

$$N_i = (1 - d)N_{i-1} + bN_{i-1-k} \quad (39)$$

If b and d are constants, then the solution is given by

$$N_i = \sum_{j=1}^{k+1} A_j \lambda_j^i \quad (40)$$

where λ_j ($1 \leq j \leq k+1$) are the roots of the polynomial equation

$$\lambda^{k+1} = (1 - d)\lambda^k + b \quad (41)$$

A_j , $1 \leq j \leq k+1$, are constants which need to be selected properly to satisfy the $(k+1)$ initial conditions.

6.3 Computational Methods

Difference equations are ideally suited for solution on digital computers. The alternative representation - i.e. reformulating a higher-order equation as a vector first-order equation (as indicated in Section 4.2 of Chapter 5), is desirable, as it results in the formulation being transformed into a first-order recursive relationship.

7 Ordinary Differential Equation (O.D.E.) Formulations

This class of formulations was discussed in Section 5 of Chapter 5. A general n th-order initial value formulation is given by

$$D^{(n)}z(t) = g\{D^{(j)}z(t), 0 \leq j \leq n-1; D^{(j)}u(t), 0 \leq j \leq m; \theta(t)\} \quad (42)$$

where D is the derivative operator ($D^{(j)} = d^j/dt^j$ and $D^{(0)}z(t) = z(t)$) and the initial condition specified through $z(t)$ and its first $(n-1)$ derivatives at $t=0$.

7.1 Analytical Methods

As in the case of difference equation formulations, only for a small class of O.D.E. formulations can an analytical solution be obtained. One such is when the equation is linear and the parameters time-invariant. For some special cases of non-linear equations it is possible to obtain analytical solutions by employing ingenious methods.

7.2 Case Study E [Cont.] (World Population)

In Section 5.5 of Chapter 5 we formulated three models (Models E.4 to E.6) involving O.D.E. formulations.

MODEL E.4

The model is given by

$$N'(t) = \alpha N(t) \quad (43)$$

with $N(t)$ representing total population at time t and

$$\alpha = b - d \quad (44)$$

with b and d being the birth and death rates respectively. Let N_0 represent the initial population at $t = 0$.

Since b and d are constants, the equation is linear and the solution given by

$$N(t) = N_0 e^{-\alpha t} \quad (45)$$

As in the case of Model E.1, the solution either increases or decreases monotonically with t , or else remains constant depending on α .

MODEL E.6

Consider the model given by the following coupled non-linear O.D.E. formulation:

$$\left. \begin{aligned} N'_m(t) &= -d_m N_m(t) + \alpha \sqrt{N_m(t) N_f(t)} \\ N'_f(t) &= -d_f N_f(t) + (1 - \alpha) \sqrt{N_m(t) N_f(t)} \end{aligned} \right\} \quad (46)$$

To obtain the solution, we define two variables $n_m(t)$ and $n_f(t)$ as follows.

$$N_m(t) = n_m^2(t) \quad \text{and} \quad N_f(t) = n_f^2(t) \quad (47)$$

On substituting (47) into (46) we have

$$\left. \begin{aligned} n'_m(t) &= -d_m n_m(t) + \alpha n_f(t) \\ n'_f(t) &= -d_f n_f(t) + (1 - \alpha) n_m(t) \end{aligned} \right\} \quad (48)$$

which is a system of linear O.D.E.s. This can be solved analytically to obtain $n_m(t)$ and $n_f(t)$, and from this $N_m(t)$ and $N_f(t)$ can be obtained using (47). (Note that, in the above procedure, we transformed non-linear equations into linear equations by a suitable transformation.)

7.3 Approximate Analytical Methods

It is often either impossible, or extremely difficult, to obtain an exact analytical solution. However, it is sometimes possible to obtain an approximate analytical solution which is close to the true solution in some sense. The approximate analytical solution is obtained by solving either a simpler formulation or a series of simpler formulations to improve the accuracy of the approximate analytical solution. In this context, various techniques have been developed – e.g. asymptotic expansion, regular perturbation, singular perturbation, to name a few. We illustrate the use of the regular perturbation technique to obtain an approximate solution by considering Case Study D.

7.3.1 REGULAR PERTURBATION TECHNIQUE

This technique is applicable if the formulation has a small parameter. Consider an O.D.E. formulation of the form

$$x'(t) = F(x(t), \varepsilon) \quad (49)$$

where $0 < \varepsilon \ll 1$. The solution $x(t)$ depends on ε and can be expressed in the form

$$x(t) = x(t, \varepsilon) = \sum_{i=0}^{\infty} X_i(t) \varepsilon^i \quad (50)$$

Since ε is small, by ignoring terms with $i > I$, we obtain an approximate solution $x_a(t)$ given by

$$x_a(t) = \sum_{i=0}^I X_i(t) \varepsilon^i \quad (51)$$

The error between $x(t)$ and $x_a(t)$ is $O(\varepsilon^I)$ and hence by choosing I properly the error can be made as small as desired. Note that we obtain a family of approximate solutions by varying I .

The functions $X_i(t)$, $i \geq 0$, are obtained by substituting (50) into (49); carrying out a power series expansion in ε and solving the equations obtained from setting the coefficient of ε^i , $i \geq 0$, to zero.

If ε appears as the coefficient of the derivative – i.e. the formulation is of the form

$$\begin{aligned} \varepsilon x'_1(t) &= F_1(x_1(t), x_2(t)) \\ x'_2(t) &= F_2(x_1(t), x_2(t)) \end{aligned} \quad (52)$$

then the above technique fails, and in this case we need to use singular perturbation techniques. Formulations of the type indicated in (52) arise when there are several widely separated time scales in the system.

7.4 Case Study D [Cont.] (Rocket Launch)

In Section 4.2 we showed that, by using grouping 3, the model for the rocket launch is given by

$$y''(\tau) = d^2 y(\tau) / d\tau^2 = -1 / (1 + \varepsilon y(\tau))^2 \quad (53)$$

with

$$y(0) = 0 \quad \text{and} \quad y'(0) = 1 \quad (54)$$

and the variables $y(\tau)$ and τ related to the original variables $x(t)$ and t as indicated in (10). If $V^2 \ll g_0 R$ then $\varepsilon \ll 1$, in which case we can obtain approximate analytical solutions using the regular perturbation technique. As

such, we assume the solution to be of the form

$$y(\tau) = y(\tau, \varepsilon) = \sum_{i=0}^{\infty} \varepsilon^i y_i(\tau) \quad (55)$$

and substituting in (53) yields,

$$\sum_{i=0}^{\infty} \varepsilon^i d^2 y_i(\tau)/d\tau^2 = -\{1 + \varepsilon \sum_{i=0}^{\infty} \varepsilon^i y_i(\tau)\}^{-2}. \quad (56)$$

On expanding the right-hand side in a power series and equating the coefficients of ε^0 we have

$$d^2 y_0(\tau)/d\tau^2 = -1 \quad (57)$$

$$y_0(0) = 0 \quad y'_0(0) = 1$$

This yields the first approximate solution $y_a(\tau)$ given by

$$y_a(\tau) = y_0(\tau) = \tau - \tau^2/2 \quad (58)$$

The error between $y_a(\tau)$ and $y(\tau)$ is $O(\varepsilon)$.

To obtain a more accurate solution we evaluate $y_1(\tau)$. By equating the coefficients of ε^1 in (56) we have

$$d^2 y_1(\tau)/d\tau^2 = -2y_0(\tau) \quad (59)$$

$$y_1(0) = y'_1(0) = 0$$

Using $y_0(\tau)$ from (58) in (59) we have

$$y_1(\tau) = \{\tau^3/6 - \tau^4/24\}. \quad (60)$$

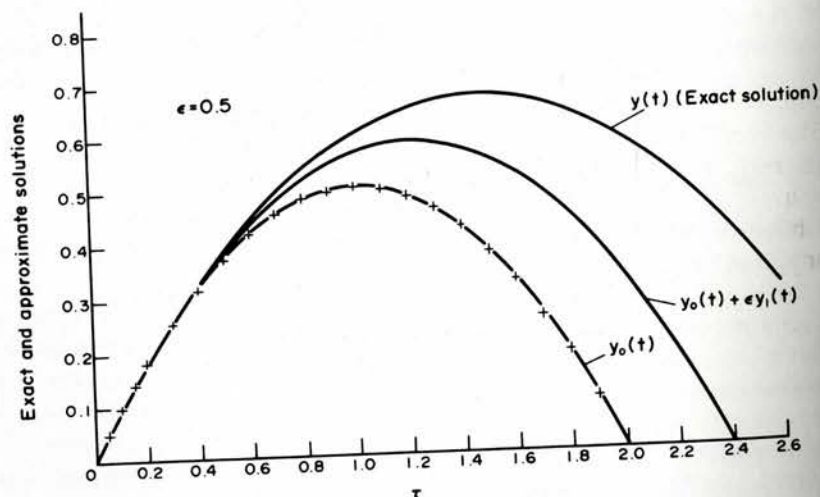


FIGURE 6.1 Exact and approximate solutions, Case Study D.

The second approximate solution $y_a(\tau)$ given by

$$y_a(\tau) = \tau - \tau^2/2 + \varepsilon\{\tau^3/6 - \tau^4/24\} \quad (61)$$

is accurate to $O(\varepsilon^2)$. By evaluating $y_i(\tau)$, $i \geq 2$, the accuracy of the approximate solution can be improved.

Plots of $y_a(\tau)$ obtained by (58) and (61) are shown in Figure 6.1 for $\varepsilon = 0.5$.

7.5 Computational Methods

As indicated in Section 5.2 of Chapter 5, an n th-order O.D.E. formulation can be reduced to a vector first-order O.D.E. formulation. Hence, without loss of generality we can confine our attention to solving vector first-order equation formulations. Let the equation be given by

$$X'(t) = F(X(t)) \quad (62)$$

Solutions for this on a digital computer can only be obtained for discrete values of t . Let X_i represent the computed solution for $t = t_i$ and $X(t_i)$ the true exact solution.

A variety of methods are available for computing X_i . These can be divided into:

- (i) *single-step methods* – if X_i is obtained using only X_{i-1} ; and
- (ii) *multi-step methods* – if X_i is obtained using X_{i-k} ; $1 \leq k \leq K$ with $K > 1$.

Single-step methods are self-starting, whilst multi-step methods require some single-step method to initiate.

Each of the above two methods can be further subdivided into explicit methods and implicit methods. Explicit methods do not involve $F(X_i)$ to obtain X_i , while implicit methods do. As a result, for implicit methods an iterative scheme is needed to solve a system of non-linear algebraic equations to obtain X_i if the function $F(X)$ is non-linear. The advantage of implicit methods over explicit methods is that they are more stable, but they require greater computation per step.

The step size $h_i = t_i - t_{i-1}$ plays an important role. The error between the computed solution and the exact solution is a function of the step sizes used and the order of the method. For a p th-order method with fixed step size h , the error $\sim O(h^{p+1})$.

If the equation to be solved is "stiff", i.e. some components of $X(t)$ change slowly while others change rapidly, then one needs to use highly stable methods. Again a variety of methods have been developed, some of which require not only the evaluation of the function $F(X)$ but also the Jacobian $J(X)$ ($= \partial F(X)/\partial X$) at each step.

Most mathematical software packages contain a variety of subroutines for solving initial value O.D.E. formulations by different methods. Many have automatic step size control. This allows for the step size to be varied so as to

ensure that the local error (either absolute or relative) is always less than some pre-specified limit. Some have special features which stop computation when some function of the solution becomes zero, or a component of the solution reaches some specified value.

7.6 Case Study D [Cont.] (Rocket Launch)

In Section 7.4 we obtained two approximate solutions, given by equations (58) and (61), for $y(\tau)$. In this section we present the solution to the full (exact) equation by using sub-routine D02BGF from the NAG package.* The reason for using this subroutine is that the computations can be stopped once the velocity changes from positive to negative, indicating that the peak altitude has been reached.

The model equation is given by (53), and in order to use the subroutine this needs to be written as a system of first-order equations. Towards this end, we define x_1 and x_2 as follows:

$$x_1(\tau) = y(\tau), \quad x_2(\tau) = y'(\tau) \quad (63)$$

Then (53) can be re-written as

$$\left. \begin{aligned} x_1'(\tau) &= x_2(\tau) \\ x_2'(\tau) &= -1/(1 + \varepsilon x(\tau))^2 \end{aligned} \right\} \quad (64)$$

A plot of $y(\tau)$ for $\varepsilon = 0.5$ is given in Figure 6.1, and can be compared with the approximate solutions obtained using the regular perturbation technique. Figure 6.2 gives the digitally computed solution for a range of ε .

7.7 Solution of O.D.E. (Boundary Value Formulations)

We shall confine our attention to two-point boundary value formulations (t.p.b.v.f.) as these arise in the solution of partial differential equations. A general t.p.b.v.f. is given by

$$x' = f(x, u, t) \quad t_0 \leq t \leq t_f \quad (65)$$

where x is a n -dimensional vector, $u(t)$ a specified function and the boundary conditions are specified in terms of n_1 functions ($g_1 = 0$) at $t = t_0$ and ($n - n_1$) functions ($g_2 = 0$) at $t = t_f$, i.e.

$$\left. \begin{aligned} g_1(x(t_0), t_0) &= 0 \quad (n_1 \text{ dimensional}) \\ g_2(x(t_f), t_f) &= 0 \quad (n - n_1 \text{ dimensional}) \end{aligned} \right\} \quad (66)$$

It is assumed that the boundary conditions ensure a unique solution.

*NAG is a package developed by the Numerical Algorithms Group. D02BGF uses a Runge-Kutta-Merson method which stops computing when a specified component of $x(t)$ reaches some specified value.

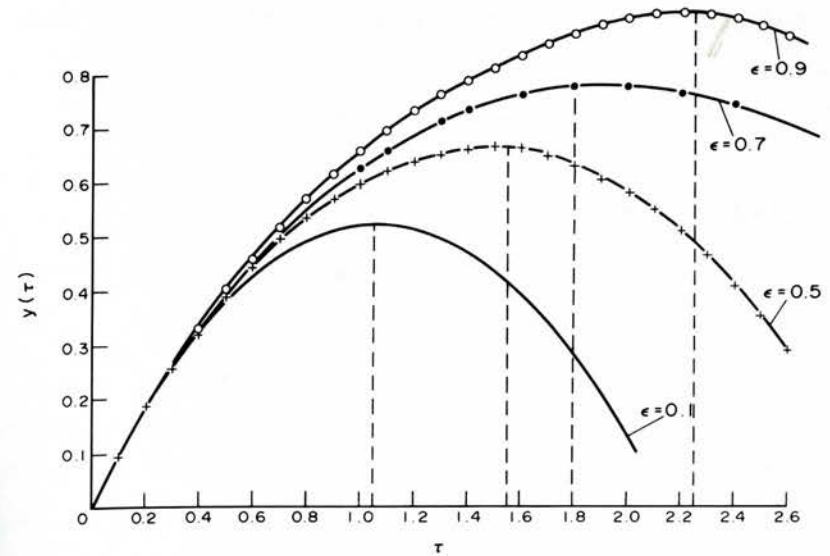


FIGURE 6.2 Plot of $y(\tau)$ vs τ for difference ε .

7.7.1 METHODS OF SOLUTION

Analytical solutions are obtainable only for a small class of formulations (e.g. linear equation formulation). A variety of methods are available for solving t.p.b.v.f. The two most important ones are:

- (i) *Transformation method*: in this method the t.p.b.v.f. is transformed into an initial value formulation – e.g. Riccati transformation for solving linear t.p.b.v.f.
- (ii) *Green's function method*: in this method the t.p.b.v.f. is transformed into an integral equation formulation.

In general, a computational procedure is needed to obtain the solution. Two methods for obtaining the solution are the following:

- (i) *Shooting method*: here the missing ($n - n_1$) conditions at t_0 are guessed, and the equation solved as an initial value formulation. In general, the computed values at t_f will not satisfy the condition $g_2(x(t_f), t_f) = 0$. An iterative scheme is used where the initial conditions are altered during each iteration so as to yield the desired solution.
- (ii) *Quasi-linearization method*: in this method the non-linear t.p.b.v.f. is solved iteratively as a sequence of linear t.p.b.v.f.

Again most mathematical software packages contain a variety of subroutines for solving t.p.b.v.f. by different methods.

8 Partial Difference Equation (P.D.E.) Formulations

This class of formulation was discussed in Section 7 of Chapter 5. In this section we discuss analytical and computational methods of solving such formulations.

8.1 Analytical Methods

Only for a small class of formulations is it possible to obtain analytical solutions. One such is a linear equation formulation with fairly simple I.C. and B.C.s. A variety of techniques have been developed to produce analytic solutions for this formulation. Some of the well-known ones are: integral transform method, separation of variables and Green's function method.

8.2 Case Study F [Cont.] (River Pollution)

In Section 7.5 of Chapter 5 we formulated a model (Model F. 1) for studying the dispersion of pollution in a river.

MODEL F. 1

Assume that the velocity of flow is negligible and hence $U = 0$. As a result, the model for pollution concentration is given by

$$\partial^2 T(x, t) / \partial x^2 = (1/D) \partial T(x, t) / \partial t \quad (67)$$

with the B.C. and I.C. given by

$$\left. \begin{array}{l} \text{B.C. } T(-L_1, t) = 0 = T(L_2, t), \quad 0 \leq t < \infty \\ \text{I.C. } T(x, 0) = G(x) \end{array} \right\} \quad (68)$$

We shall use the method of separation of variables. The method assumes a solution of the form

$$T(x, t) = W(x)V(t) \quad (69)$$

Substituting this in (67) yields

$$\frac{1}{D} W(x) \frac{dV(t)}{dt} = V(t) \frac{d^2 W(x)}{dx^2} \quad (70)$$

implying

$$\frac{1}{W(x)} \frac{d^2 W(x)}{dx^2} = \frac{1}{DV(t)} \frac{dV(t)}{dt} = -\lambda^2 \quad (71)$$

As a result $W(x)$ is given by

$$W(x) = \sum_{\lambda} \{C_{\lambda} \sin \lambda(x + L_1) + D_{\lambda} \cos \lambda(x + L_1)\} \quad (72)$$

and $V(t)$ is given by

$$V(t) = e^{-D\lambda^2 t} \quad (73)$$

Since the B.C. have to be satisfied, we have $D_{\lambda} = 0$ and λ must satisfy

$$\lambda(L_1 + L_2) = n\pi; \quad n = 0, 1, 2, \dots \quad (74)$$

or

$$\lambda = n\pi / (L_1 + L_2); \quad n = 0, 1, 2, \dots \quad (75)$$

As a result, the solution is given by

$$T(x, t) = \sum_{n=0}^{\infty} \alpha_n e^{-\gamma t} \sin \left\{ \frac{n\pi(x + L_1)}{L_1 + L_2} \right\} \quad (76)$$

with

$$\gamma = Dn^2\pi^2 / (L_1 + L_2)^2 \quad (77)$$

and α_n to be selected to satisfy the I.C. From (76) we have

$$T(x, 0) = \sum_{n=0}^{\infty} \alpha_n \sin \left\{ \frac{n\pi(x + L_1)}{(L_1 + L_2)} \right\} \quad (78)$$

and for this to equal $G(x)$ we must have

$$\alpha_n = \int_{-L_1}^{L_2} G(x) \sin \left\{ \frac{n\pi(x + L_1)}{(L_1 + L_2)} \right\} dx \quad (79)$$

Thus, the analytical solution is given by (76) with α_n evaluated from (79).

8.3 Approximate Analytical Methods

As with O.D.E. formulations, approximate solutions can often be obtained by exploiting special features of the formulation, in a manner similar to O.D.E. formulations.

8.4 Computational Methods

We shall confine our discussion to formulations with two independent variables. In this case there are two different approaches that we can use to obtain a computer solution. In the first approach all the partial derivatives are replaced by appropriate finite differences. As a result the formulation is reduced to a two-dimensional difference equation which relates the dependent variables for discrete values of the two independent variables. In the second approach only the partial derivatives with respect to one independent variable are replaced by finite differences. As a consequence the formulation is reduced to a system of O.D.E.s which can be solved by methods discussed in Section 7.5. The step size used in the discretization of the independent variable affects the accuracy as well as the stability of the computational scheme. Various schemes have been developed for solving specific types of P.D.E. formulations.

8.5 Case Study E [Cont.] (World Populations)

In Section 7.4 of Chapter 5 we formulated a model (Model E.8) for population changes involving a first-order partial differential equation formulation.

MODEL E.8

The model is given by

$$\frac{\partial N(x, t)}{\partial t} + \frac{\partial N(x, t)}{\partial x} = -d(x)N(x, t) \quad (80)$$

with

$$N(0, t) = \int_0^{x_m} b(x)N(x, t) dx \quad (81)$$

and the I.C. by

$$N(x, 0) = G(x) \quad (82)$$

(Note that the domain for $N(x, t)$ is given by $0 \leq x \leq x_m$ and $t \geq 0$.)

Let $t_i, i = 0, 1, 2, \dots$, be a sequence of points equi-spaced along the t axis with $t_i = ih$ and h being a small positive quantity. Replacing the partial derivative with respect to t by a first-order backward difference, i.e.

$$\frac{\partial N(x, t)}{\partial t} \approx \frac{N(x, t_i) - N(x, t_{i-1})}{h} \quad (83)$$

and using the notation $N_i(x)$ for $N(x, t_i)$, (80) gets reduced to a system of O.D.E.s given by

$$dN_i(x)/dx + [(1/h) + d(x)]N_i(x) = (1/h)N_{i-1}(x) \quad (84)$$

and

$$N_i(0) = \int_0^{x_m} b(x)N_i(x) dx \quad (85)$$

for $i = 1, 2, \dots$

This system of O.D.E. equations can be solved recursively as

$$N_0(x) = N(x, 0) = G(x) \quad (86)$$

is known. Since $N_i(0)$ depends on $N_i(x)$, $0 \leq x \leq x_m$, an iterative technique will be needed to obtain $N_i(x)$ given $N_{i-1}(x)$. One such technique is to guess $N_i(0)$ and obtain $N_i(x)$ by solving (84). Using this computed solution the integral in (85) can be computed and compared with the guessed value of $N_i(0)$. If the two are not the same, the guessed value is modified and the procedure repeated till (85) is satisfied.

Notes and References

The appeal and the use of analog and hybrid computers to solve mathematical formulations have diminished considerably due to developments in digital computers and mathematical software since 1970. As a consequence, there have been no recent books on analog or hybrid computers. [1] and [2] are two of the most recent books on these computer types. In contrast, the list of books on digital computers and digital computing is not only very large, but continues to grow at an exponential rate; [3]–[5] show a small sample.

For more on dimensional analysis, see [6]; on simplification and scaling, see [7]. Item [8] deals with scale effects in animal locomotion. Books on analog computing contain a detailed discussion on scaling of differential equations.

Numerical and computational techniques for solving static optimization models have received a lot of attention. Books on this topic vary from general (e.g. [9]–[11]) to those giving an in-depth study of a particular method (e.g. [12]) or type (e.g. [13] and [14]). Most elementary books on numerical analysis or methods (e.g. [15]–[17]) contain one or more chapters on solving linear and non-linear algebraic equations.

Books on ordinary differential equations (e.g. those cited in Chapter 7) discuss both exact and approximate analytical methods of solutions. Item [18] deals with the use of similarity methods in solving, and [19] is one of many books which discuss solving differential equations using physical understanding. The number of books on approximate methods of solution is also large. Some of these are general (e.g. [20]) while others deal with specific techniques (e.g. [21] and [22]). Items [23]–[25] are a small sample of books on numerical methods for solving differential equations.

Most books on partial differential equations discuss a variety of analytical solution techniques. See the list at the end of Chapter 5 for a short selection of such books. Numerical methods of solution is an active area of research and new schemes are constantly being developed. Books on numerical methods can be divided into two categories. Those belonging to the first category are of a general nature (e.g. [26]–[29]) while those belonging to the second deal with a particular method or type of formulation (e.g. [30]).

NAG and IMSL are two fairly well-known software packages which contain a large number of programs for solving a variety of mathematical formulations. For further details see [31] and [32].

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CHAPTER 7

Mathematical Formulations – II

1 Introduction

In Chapter 5 we discussed mathematical formulations suitable for modelling deterministic systems. When uncertainty is a significant feature of the system, the system characterization must be done in a stochastic framework. As a consequence the mathematical formulations which can be used as dummies in the modelling must allow the variables to change in an unpredictable fashion, so that they adequately model the uncertainty of the system when the formulation becomes a model. Such formulations belong to the theory of probability and stochastic processes.

In this chapter we discuss some of the mathematical formulations from the theory of probability and stochastic processes that are suitable for use as dummies in modelling systems that involve uncertainties. We commence with a brief discussion of random variables and general stochastic processes. Following this, we discuss the different types of mathematical formulations that are available for modelling systems with uncertainty. Later, we examine some of these formulations individually. For each formulation we give a brief introduction to the general structure, discuss some important features and finally illustrate their use as dummies in modelling one or more of the case studies discussed in Chapter 2 using the system characterization done in Chapter 3.

2 Random Variable and Stochastic Process

A random variable $X(\omega)$ can be viewed as a function which assigns a number to every outcome ω of an experiment. The domain of $X(\omega)$, Ω , is the set of all experimental outcomes (ω) and range, R , the set of real numbers. Since the outcome of an experiment is uncertain, the value assumed by $X(\omega)$ is also uncertain.

A rigorous approach to characterizing $X(\omega)$ would commence with an axiomatic characterization of Ω ; the probability measures on sets of outcomes

belonging to Ω and $X(\omega)$ defined as a set function. An alternative characterisation of $X(\omega)$ is through a distribution function $F(x, \theta)$ with

$$F(x, \theta) = \text{prob}\{X(\omega) \leq x\}, -\infty < x < \infty, \quad (1)$$

and $F(x, \theta)$ being a non-decreasing function in x , with $F(-\infty, \theta) = 0$ and $F(+\infty, \theta) = 1$ and θ being a set of parameters. If $X(\omega)$ is n -dimensional, then it is characterized by a n -dimensional distribution function of the form

$$F(x_1, x_2, x_3, \dots, x_n; \theta) = \text{prob}\{X_1(\omega) \leq x_1, \dots, X_n(\omega) \leq x_n\} \quad (2)$$

where $X_1, X_2, \dots, X_n$ are the components of the vector $X(\omega)$.

A stochastic process can be viewed as an extension of a random variable in the sense that it can be viewed as a function of two variables t and ω and of the form $X(t, \omega)$. The independent variable t assumes real values in an interval T (either finite or infinite) and corresponds to time when the process is used to model dynamic systems with uncertainty and ω represents the uncertain outcome and belongs to a set Ω . For a given $t \in T$, $X(t, \omega) = X(\omega)$ is a random variable taking on values in the range R , the set of real numbers. For a given $\omega \in \Omega$, $X(t, \omega) = x(t)$ is an outcome or realization of the process; i.e. it is a function of the independent variable t .

A general stochastic process $X(t)^*$ can be characterized either axiomatically or through an alternative approach involving joint distribution functions. Let $t_1 < t_2 < \dots < t_{n-1} < t_n$ ($t_i \in T$, $1 \leq i \leq n$) be n arbitrary points. Then the distribution function

$$F(x_1, t_1; x_2, t_2; \dots; x_n, t_n) = \text{prob}\{X(t_1) \leq x_1, X(t_2) \leq x_2, \dots, X(t_n) \leq x_n\} \quad (3)$$

characterizes $X(t, \omega)$ for n values of t . If the values assumed by t are infinite, then we need to characterize the distribution function with $n \rightarrow \infty$. This makes the process unmanageable and of limited use in modelling. This difficulty is overcome by requiring the process to have the Markov property.

2.1 Markov Property

A stochastic process $X(t)$ is said to have the Markov property if, for $t_1 < t_2 < t_3 < \dots < t_{n-1} < t_n$, ($t_i \in T$, $1 \leq i \leq n$), we have

$$\begin{aligned} \text{prob}\{X(t_n) \leq x_n | X(t_1) = x_1, \dots, X(t_{n-1}) = x_{n-1}\} \\ = \text{prob}\{X(t_n) \leq x_n | X(t_{n-1}) = x_{n-1}\} \end{aligned} \quad (4)$$

In this case the n -dimensional distribution functions characterizing

* We shall use $X(t)$ instead of $X(t, \omega)$ so as to simplify the notation. $x(t)$ is a deterministic function representing an outcome of $X(t)$. $x_1 \dots x_n$ are deterministic quantities, and represent outcome of $X(t)$ at $t = t_1, t_2, \dots, t_n$.

$\{X(t_1), X(t_2), \dots, X(t_n)\}$ for $n > 2$, can be written as a product of two-dimensional conditional distribution functions of the form $F(x_i, t_i | x_{i-1}, t_{i-1})$. Thus the process is completely characterized by specifying the two-dimensional joint distribution function $F(x_i, t_i; x_j, t_j)$ for all $t_i, t_j \in T$.

Stochastic processes having the Markov property are called Markov processes; otherwise they are called non-Markov processes.

3 Types of Formulations

Broadly speaking, the mathematical formulations suited for modelling uncertain systems can be divided into two categories:

- (1) static formulations
- (2) dynamic formulations.

3.1 Static Formulations

Static formulations are mathematical formulations involving algebraic equations or functions with one or more of the variables being random. The variables can be either scalars or vectors, either discretely or continuously valued and either constrained or unconstrained. When the formulation becomes a mathematical model, there is a one-to-one correspondence between variables of the formulation and the physical variables of the system characterization. Such formulations are suited for modelling uncertain static systems.

3.2 Dynamic Formulations

Dynamic formulations are mathematical formulations involving stochastic processes with the independent variable t representing time when the formulation is used to model uncertain dynamic systems. The variables are of the form $X(t, \omega)$ and, as discussed earlier, the formulations can be divided into two types - Markov or non-Markov - based on whether the process $X(t, \omega)$ has the Markov property or not.

Each of the above two types can be divided into four subtypes based on:

- (1) the values assumed by the process $X(t)$ ($\equiv X(t, \omega)$) being discrete or continuous; and
- (2) the values assumed by the independent variable t being discrete or continuous,

and is as shown below:

		<i>t</i>	
		Discrete	Continuous
<i>X</i>	Discrete	D ₁	D ₂
	Continuous	D ₃	D ₄

D1: DISCRETE STATE/DISCRETE TIME FORMULATIONS

In this both $X(t)$ and t assume only discrete values. Let the values assumed by $X(t)$ be denoted by $s_1, s_2, \dots, s_r$, called the states of the process. The integer r can be either finite or infinite. The values assumed by t are denoted by $t_1, t_2, \dots$ which form an increasing sequence.

If the process is Markovian and r is finite, then the formulation is called a Markov chain. If the process is Markovian and $r \rightarrow \infty$, then the formulation is called a Markov chain with infinite states.

D2: DISCRETE STATE/CONTINUOUS TIME FORMULATIONS

In this $X(t)$ assumes only discrete values $s_1, s_2, \dots, s_r$ and t assumes a continuous range of values in an interval T which can be either finite or infinite.

If the process is Markovian, then it is called a continuous time Markov chain formulation.

D3: CONTINUOUS STATE/DISCRETE TIME FORMULATIONS

In this $X(t)$ assumes a continuous range of values (i.e. continuous state space) and t assumes only discrete values. Such a formulation is also called a stochastic sequence, and if the process is Markovian, then it is also called Markov sequence formulation.

D4: CONTINUOUS STATE/CONTINUOUS TIME FORMULATIONS

In this, both $X(t)$ and t assume a continuous range of values. If the process is Markovian, then it is called a continuous time Markov process formulation. This type of formulation can be further subdivided, and we discuss this in a later section.

3.3 Stationary vs Non-stationary Process

A process $X(t)$ (Markovian or non-Markovian), is said to be stationary if the distribution function is invariant under a shift in t ; i.e.

$$F(x_1, t_1; x_2, t_2; \dots; x_n, t_n) = F(x_1, t'_1; x_2, t'_2; \dots; x_n, t'_n) \quad (5)$$

with $t'_i = t_i + \tau$ ($1 \leq i \leq n$) for all τ and n .

For a Markov process, stationarity implies that the two-dimensional distributions function has the form

$$F(x_i, t_i; x_j, t_j) = F(x_i, x_j, \tau) \quad (6)$$

where $\tau = t_j - t_i$ (we have assumed that $t_j > t_i$).

3.4 Second-order Characterization

A second-order characterization involves only the first and second moments of $X(t)$, and is given by the following two functions:

$$m(t) = E[X(t)], (t \in T) \quad (7)$$

$$R(t, t') = E[\{X(t) - m(t)\}\{X(t') - m(t')\}], (t, t' \in T) \quad (8)$$

If the process is stationary, then $m(t) = m$ and $R(t, t') = R(t - t')$, i.e. the first moment is a constant and the second moment is a function of only one variable, $\tau = t - t'$.

In general, a second-order characterization contains less information about $X(t)$ than a characterization involving the distribution functions. However, when $X(t)$ is Gaussian, the two characterizations are equivalent.

4 Static Formulations

As mentioned earlier, static formulations involve algebraic equations with one or more of the variables being random. In this section we discuss two such formulations.

4.1 Analysis of Variance Formulation

Such formulations are used extensively in many disciplines for modelling experimental situations involving one or more factors which have some effect on the observations. The formulations relate the observed values to the effect of these factors. The effects are two types:

- assignable effects which result from recognizable conditions, and
- unassignable effects which result from unrecognizable and random conditions.

The model formulation is of the form:

$$\text{observed value} = \sum \{\text{parameters representing assignable effects}\} + \sum \{\text{random variables representing assignable effects}\} + \sum \{\text{random variables represent unassignable (residual) effects}\}$$

We shall illustrate the use of such formulations in solving problems by considering Case Study B.

4.2 Case Study B [Cont.] (Alloy Selection)

The system characterization for this problem was done in Chapter 3, Section 6.2. The variable of interest is the thermal coefficient of the alloy and the two factors are the variations of ore from mines and the methods of manufacture. Let n specimens (or samples) be obtained for each combination of ore and method of manufacture.

The first factor, viz. the mine from which the ore is obtained, can be viewed as a four-level factor, where the term "level" is used to describe a particular property defining each category of the factor. Level i corresponds to MA_i (i.e. ore from mine i), $1 \leq i \leq 4$. Similarly, the second factor, viz. method of manufacture, is a two-level factor with level j corresponding to method ME_j , $1 \leq j \leq 2$.

Such a situation corresponds to what is known as the "analysis of two-factor cross-classification model" in the general theory of the analysis of variance formulations.

MODEL B.1

Using the notation of the system characterization, we have TC_{ijk} to represent the thermal coefficient of the k th specimen produced using ore from mine i , i.e. MA_i and method ME_j . The limits for the subscripts are as follows: $1 \leq i \leq 4$, $1 \leq j \leq 2$ and $1 \leq k \leq n$.

We assume that the effect of the two factors on the thermal coefficient TC_{ijk} to be of the form

$$TC_{ijk} = A + R_i + C_j + (RC)_{ij} + X_{ijk} \quad (9)$$

where we have the set of parameters given by $\{A, R_i (1 \leq i \leq 4), C_j (1 \leq j \leq 2)$ and $(RC)_{ij} (1 \leq i \leq 4, 1 \leq j \leq 2)\}$ which can be interpreted as follows:

- A : the overall average,
- R_i : the average deviation in A due to i th level of first factor,
- C_j : the average deviation in A due to j th level of second factor,
- $(RC)_{ij}$: the average deviation in A due to interaction between the i th level of first factor and the j th level of second factor,
- X_{ijk} : residual term representing the unassignable (and random) effects.

Because R_i , C_j and $(RC)_{ij}$ represent average deviations from the overall average A , we have the following set of constraints.

$$\sum_{i=1}^4 R_i = 0, \quad \sum_{j=1}^2 C_j = 0$$

$$\sum_{i=1}^4 (RC)_{ij} = 0 \quad 1 \leq j \leq 2 \quad (10)$$

$$\sum_{j=1}^2 (RC)_{ij} = 0 \quad 1 \leq i \leq 4 \quad (11)$$

(Note: If we ignore the term $(RC)_{ij}$ in (9) we are ignoring the interaction between the effects of the two factors, and in this case we have a simpler model which is called the "additive" model.)

We assume that these residual (random) terms are characterized as follows:

- (i) $E[X_{ijk}] = 0$ for all i, j and k ,
- (ii) X_{ijk} are mutually independent,
- (iii) $\text{var}[X_{ijk}] = \sigma^2$ for all i, j and k
- (iv) X_{ijk} is normally distributed.

To decide whether a particular combination of method and mine ore has any significant influence on the thermal coefficient of the alloy can be done by testing the null hypothesis that $(RC)_{ij} = 0$ for all i and j against an alternative hypothesis that at least one of them is different from zero. Similarly, we can decide whether the method of manufacture has significant influence or not, and so on.

4.3 Regression Formulations

The typical form for such formulations is given by an equation

$$Y = g(X_1, X_2, \dots, X_n, \theta) + V \quad (12)$$

where $X_i (1 \leq i \leq n)$ are known variables, V an unknown random variable and Y another known variable. The structure of the formulation is given by the function g , and θ is the set of model parameters.

Such formulations are useful for modelling uncertain systems with "black-box" characterization, with $X_i (1 \leq i \leq n)$ representing the system input variables, Y the system output variable and V representing uncertainty in the system.

Without loss of generality we can assume that the mean of V is zero. As a part of specifying the formulation one needs to specify the distribution function $F(v)$ for the random variable V .

Regression formulations are often used for modelling uncertain dynamic systems by letting one of the known variables X_i , $1 \leq i \leq n$, to represent the independent variable time. An alternative approach is by indexing the variables and the indexing linked to time. In other words, the formulation is of the form

$$Y_i = g(X_{1i}, X_{2i}, \dots, X_{ni}, \theta) + V_i \quad (13)$$

with Y_i representing $Y(t)$ at time $t = t_i$ and so on. Note that, in (13), the relationship involves variables at a single discrete time instant t_i only. Thus there is no memory effect, as the formulation does not involve past values of the variables. If the relationship involves variables at more than one time instant (say X_{1i} and X_{1j} , $i > j$) then the formulation models memory effects. The sequence V_i in (13) can be either independent or correlated.

Regression formulations can be divided into two types – linear and non-linear. If the variables X_i ($1 \leq i \leq n$) appear linearly in g then it is a linear regression formulation; if not, the formulation is non-linear.

4.4 Case Study J [Cont.] {Speed of Aeroplanes}

The system characterization for this problem was done in Chapter 3, Section 6.10, and the problem is to obtain forecasts for the maximum speed of aeroplanes for the year 2000. In this section we develop a sequence of models involving regression formulations. We employ the notation used in the system characterization – i.e. $X(t)$ represents the maximum speed achieved at time t . The time variable t is continuously valued with $1900 \leq t < \infty$, since $X(t) = 0$ for $t < 1900$.

MODEL J.1 (Linear Regression)

We assume that the maximum speed achieved at time t ($t \geq 1900$) is given by

$$X(t) = a_1 + b_1(t - 1900) + V(t) \quad (14)$$

where a_1 and b_1 are non-negative constants, $V(t)$ is a random process with zero mean, variance σ^2 and $V(t)$ statistically independent of $V(t')$ for $t \neq t'$.

The above formulation implies that the maximum speed achieved consists of two components – one deterministic, which increases linearly with time, and the other stochastic. Note that for discrete values of t , (14) reduces to (13) since V_i in (13) corresponds to $V(t)$ for $t = t_i$ and so on.

In the above formulation the deterministic component increases linearly with time. When this assumption is not justified, we need to look at non-linear formulations. Two models involving non-linear formulations are shown below.

MODEL J.2 (Non-linear Regression)

Model J.2(a)

$$X(t) = a_2 e^{b_2(t - 1900)} + V(t) \quad (15)$$

where a_2 and b_2 are non-negative constants and $V(t)$ is as in Model J.1. In this model t appears non-linearly in the formulation.

Model J.2(b)

$$\log X(t) = a_3 + b_3(t - 1900) + V(t) \quad (16)$$

where a_3 and b_3 are non-negative constants and $V(t)$ is as in Model J.1. In this model $X(t)$ appears non-linearly.

The advantage of Model J.2(b) is that by defining

$$Y(t) = \log X(t) \quad (17)$$

(16) reduces to a linear regression formulation of form given by (14), with the parameters also appearing linearly. The same is not true for Model J.2(a).

MODEL J.3

This is a refinement of Model J.1, in the sense that it incorporates changes in technology; i.e. from piston driven to jet propulsion to rocket. More specifically, we assume the following:

- (a) For the period (1900–1940) the speed is given by

$$X(t) = c_1 + d_1(t - 1900) + V(t) \quad (18)$$

with two parameters c_1 and d_1 . This period corresponds to piston-driven engines.

- (b) For the period (1940–1980) the speed is given by

$$X(t) = c_2 + d_2(t - 1940) + V(t) \quad (19)$$

with two parameters c_2 and d_2 , and $d_2 > d_1$ indicating an increase in the rate of change due to jet engine technology replacing the earlier piston engine technology.

Note that c_2 is to be selected such that (18) and (19) yield the same value for $t = 1940$. We assume that $d_2 = 5d_1$ and later check the validity of the assumption.

- (c) For the period (1980–2020) the speed is given by

$$X(t) = c_3 + d_3(t - 1980) + V(t) \quad (20)$$

with two parameters c_3 and d_3 , and $d_3 > d_2$ indicating a faster rate of change due to rocket engine technology replacing the jet engine technology.

c_3 is to be selected such that (19) and (20) yield the same value for $t = 1980$ and we assume that $d_3 = 3d_2$ (or equivalently $= 15d_1$).

In other words, in this model the total time interval is divided into three regions, each of 40 years duration, and that the rate of growth is separate for each period because of different technologies involved. In (18)–(20) $V(t)$ is as indicated in Model J.1.

5 Discrete State/Discrete Time Formulations

Let the discrete values (or states) assumed by $X(t)$ be denoted by $s_1, s_2, \dots, s_r$ with r either finite or infinite. Similarly, let $t_0, t_1, t_2, \dots$ be the discrete values assumed by the independent variable t , with the sequence $t_i, i \geq 0$ being an increasing sequence. By suitable time scaling we can assume, without loss of generality, that the sequence $t_i, i \geq 0$ correspond to set of integers $i = 0, 1, 2, \dots$. We also use the notation $X(t)$ and X_i interchangeably.

5.1 Markov Formulations

The Markov property was discussed in Section 2.1. Formulations with this property imply

$$\begin{aligned} \text{prob} \{X_{t+1} = s_k | X_t = s_j, \dots, X_{t-k} = s_l, \dots, X_0 = s_m\} \\ = \text{prob} \{X_{t+1} = s_k | X_t = s_j\}, \quad 1 \leq j, k, l, m \leq r. \end{aligned} \quad (21)$$

As a result, for each time $t (t = 0, 1, 2, \dots)$ the formulation is completely specified by an $r \times r$ one-step transition matrix $P(t)$, with

$$P(t) = \begin{bmatrix} P_{11}(t) & \dots & P_{1r}(t) \\ P_{r1}(t) & \dots & P_{rr}(t) \end{bmatrix} \quad (22)$$

where

$$P_{jk}(t) = \text{prob} \{X_{t+1} = s_k | X_t = s_j\}, \quad (1 \leq j, k \leq r) \quad (23)$$

and subject to the following constraints.

$$\begin{aligned} \text{(i)} \quad P_{jk}(t) \geq 0, \quad 1 \leq j, k \leq r \\ \text{(ii)} \quad \sum_{k=1}^r P_{jk}(t) = 1, \quad 1 \leq j \leq r \end{aligned} \quad (24)$$

If $P(t)$ does not change with t , i.e. $P(t) = P$ for all t , then the formulation is stationary in the sense described earlier.

The one-step transition matrix characterizes the evolution of X_t (in a probabilistic sense) once the initial state of X_0 is characterized. If the state of X_0 is not known exactly, then it needs to be specified through a probabilistic characterization. This is done by an r -dimensional initial vector $p(0)$,

$$p(0) = [p_1(0), p_2(0), \dots, p_r(0)]^T \quad (25)$$

with

$$p_i(0) = \text{prob} \{X_0 = s_i\}, \quad 1 \leq i \leq r \quad (26)$$

and

$$p_i(0) \geq 0, \quad 1 \leq i \leq r; \quad \sum_{i=1}^r p_i(0) = 1 \quad (27)$$

The evolution of $X(t)$ is given by a r -dimensional vector $p(t)$,

$$p(t) = [p_1(t), p_2(t), \dots, p_r(t)], \quad (28)$$

with

$$p_i(t) = \text{prob} \{X_t = s_i\}. \quad (29)$$

It is easily seen that $p(t)$ satisfies the linear difference equation

$$p(t+1) = P^T(t)p(t) \quad (30)$$

with $p(0)$ as specified above.

5.2 Non-Markov Formulation

In this case, X_t no longer satisfies the condition given by (21). Let

$$\begin{aligned} P\{X_{t+1} = s_p | X_t = s_j, \dots, X_{t-k} = s_l, \dots, X_1 = s_m\} \\ = \{X_{t+1} = s_p | X_t = s_j, \dots, X_{t-k} = s_l\} \end{aligned} \quad (31)$$

where $1 \leq k, j, l, m, p \leq r$. Note that the state at time $(t+1)$ depends not only on the state at time t but also on the states at times $t-n, 1 \leq n \leq k$.

By enlarging the state space suitably, the above non-Markovian r state formulation can be transformed into a Markovian formulation with r^k states. We illustrate this by the following example:

Example 1

Let $r = 2$ and $k = 2$, i.e.:

$$\text{prob} \{X_{t+1} = s_k | X_t = s_j, X_{t-1} = s_m, \dots, X_1 = s_1\} = \text{prob} \{X_{t+1} = s_k | X_t = s_j, X_{t-1} = s_m\}. \quad (32)$$

Define a random variable Y_t as follows.

$$\begin{aligned} Y_t &= 1 \text{ if } X_t = s_1, \quad X_{t-1} = s_1, \\ &= 2 \text{ if } X_t = s_1, \quad X_{t-1} = s_2, \\ &= 3 \text{ if } X_t = s_2, \quad X_{t-1} = s_1, \text{ and} \\ &= 4 \text{ if } X_t = s_2, \quad X_{t-1} = s_2. \end{aligned}$$

Then, from (32) we have

$$\text{prob} \{Y_{t+1} = k | Y_t = j, Y_{t-1} = n, \dots, Y_1 = m\} = \text{prob} \{Y_{t+1} = k | Y_t = j\} \quad (33)$$

implying that Y_t is a Markov chain. Hence, we can carry out the analysis of the original non-Markov process $\{X_t\}$ by analysing the transformed Markov process $\{Y_t\}$.

5.3 Case Study G [Cont.] (Weather Changes)

The system characterization for this problem was done in Chapter 3, Section 6.7. The variable of interest is $N(t)$, which characterizes the weather on day t . As indicated in the system characterization, $N(t)$ changes randomly and assumes the following values:

$$\begin{aligned} N(t) &= 1 \text{ if day } t \text{ is sunny,} \\ &= 2 \text{ if day } t \text{ is partly sunny,} \\ &= 3 \text{ if day } t \text{ is cloudy,} \end{aligned}$$

i.e. the states of $N(t)$ are given by the set of integers $\{1, 2, 3\}$.

MODEL G.1

We assume that $N(t)$ has the Markov property and that the process is stationary. In this case the model is given by a one-step transition matrix P of the form given in (22) with $r = 3$ and $P_{ij}(t) = P_{ij}$ (a constant) for all t . The parameters are the nine entries of the transition matrix (viz. P_{ij} , $1 \leq i, j \leq 3$), subject to constraints given by (24). The initial state, viz. N_0 , is assumed to be specified.

MODEL G.2

We assume that $N(t)$ has the Markov property but is not stationary. In this case the one-step transition matrix changes with time over the year. We assume that the year can be divided into four seasons – summer, autumn, winter and spring. In any one season the changes to weather are modelled by a stationary Markov chain. As a result we have four different one-step transition matrices – one for each season. Let P^s, P^a, P^w and P^{sp} represent the four one-step transition matrices. Then each of these is subject to constraints given by (24) with $r = 3$, as a result of which we have 36 parameters and four equality constraints.

MODEL G.3

We assume that $N(t)$ does not have the Markov property and that the probabilistic characterization of $N(t+1)$ depends not only on $N(t)$ but on $N(t-j)$, $1 \leq j \leq k$, where k is specified. As mentioned earlier, this model uses a non-Markovian formulation which can be transformed into a model having the Markov property with an enlarged state space.

5.4 Special Case (Random Walk Formulation)

The random walk formulation is a special case of the Markov formulation discussed in Section 5.1. Here the state space is the set of integers from $-\infty$ to ∞ . If at time t , x_t is in state i , then at time $t+1$ it can either go to state $i+1$ or $i-1$, or have no change in the state. As a result the one-step transition matrix is a tri-diagonal infinite-dimensional matrix. Such formulations have been used extensively in modelling a range of physical systems.

6 Discrete State/Continuous Time Formulations

A fairly general stochastic process formulation with discrete state and continuous time is the semi-Markov process. We start this section with a brief introduction to this process. Following this we discuss a few specific formulations – examining their structure and illustrating their use in modelling some of the case studies discussed in Chapter 2.

6.1 Semi-Markov Process Formulations

As in Section 5, the discrete values (or states) assumed by $X(t)$ will be denoted by $s_1, s_2, \dots, s_r$, with r being either finite or infinite. Once the process enters state s_i ($1 \leq i \leq r$) the transition to next state s_j ($1 \leq j \leq r, j \neq i$) is uncertain and given by probability q_{ij} . These probabilities are constrained as follows:

$$q_{ij} \geq 0, q_{ii} = 0 \quad \text{for } 1 \leq i, j \leq r$$

and

$$\sum_{j=1}^r q_{ij} = 1 \quad (34)$$

Thus the transition to next state is completely characterized by an $r \times r$ matrix Q with elements q_{ij} as defined above. The duration for which the process stays in state s_i , once it enters it, is a random variable characterized by a distribution function which depends not only on the state s_i but also on the state s_j to which the process moves. Let τ_{ij} ($1 \leq i, j \leq r$) represent the non-negative random duration for which the process stays in s_i conditioned on the transition being to s_j ($1 \leq j \leq r, j \neq i$) and let $G_{ij}(t)$ be the associated distribution function. Thus, the semi-Markov process formulation is characterized by an $r \times r$ transition matrix Q and $r \times (r-1)$ distribution functions

$$G_{ij}(t) \{1 \leq i, j \leq r, i \neq j\}.$$

If the initial state $X(t_0)$ is not known exactly, then a probabilistic characterization of it needs to be specified. This is done by an r -dimensional vector $p(t_0)$ of the form given by (25) subject to constraints as given in (27), with $p_i(t_0)$ representing the probability of $X(t_0) = s_i$, $1 \leq i \leq r$.

A special case of this is when all the distribution functions $G_{ij}(t)$ $\{1 \leq i, j \leq r, i \neq j\}$ are exponentially distributed, i.e.:

$$G_{ij}(t) = 1 - \exp(-\theta_{ij}t) \quad (35)$$

then the process $X(t)$ has the Markov property and in this case the formulation is called a continuous time Markov chain formulation.

6.2 Some Specific Formulations

A variety of discrete state/continuous time stochastic formulations have been developed for modelling real systems. Some of these are special cases of the general formulation discussed in the previous subsection. We shall discuss a few of these formulations to highlight their role in modelling specific types of real systems. The formulations that we will discuss are the following.

- (1) point process formulation
- (2) queueing process formulation
- (3) renewal process formulation.

6.3 Point Process Formulations

Point process formulations deal with "events" occurring randomly in time. Examples of an "event" are a machine failing, a baby being born, and so on. The occurrence of events can be viewed as points distributed randomly along the time axis.

The characterization of point process formulations can be done in three different ways, which are related to each other. It could be done in terms of either

- (i) the distribution function for the number of events, $N(t)$, in an interval $(0, t]$; or
- (ii) the intensity function $\lambda(t)$, with $\lambda(t)\delta t$ being the probability of an event occurring in the interval $(t, t + \delta t]$; or
- (iii) the distribution function for the time interval between events.

Depending on the situation one of the above three might be better suited for modelling than the others.

The best-known point process formulation is the stationary Poisson process. For this process the intensity function $\lambda(t) = \lambda$ is a constant. Equivalently, it corresponds to $N(t)$ being distributed according to a Poisson distribution with parameter λ or the time interval between events being distributed according to an exponential distribution with parameter $(1/\lambda)$.

Some extensions to the stationary point process are:

- (i) non-stationary Poisson process – characterized by the intensity function $\lambda(t)$ changing with t ,
- (ii) doubly stochastic Poisson process – characterized by λ being a random variable (or $\lambda(t)$ being a stochastic process).

More complicated point processes have $\lambda(t)$ as a function of the time history of points occurring till time t .

We shall return to Poisson process formulations in a later section.

6.4 Queueing Process Formulations

In a queueing process formulation the process $X(t)$ represents the number of "customers" either waiting, or being serviced at time t . Examples of customers and service can be planes waiting to take off; patients waiting to see a doctor and so on. As a consequence, $X(t)$ assumes only non-negative integer values, with $X(t) = 0$ implying that there is no customer being served or waiting to be served at time t .

$X(t)$ changes whenever a customer arrives or leaves. If the customer arrival times and/or the time to service a customer are random, then $X(t)$ changes

randomly over time. The nature of change in $X(t)$ depends not only on the arrival pattern and the service times, but also on the number of servers (e.g. in the case of planes waiting to take off, it would be the number of separate runways) and the policy (e.g. first come, first served) used for servicing the customers.

Let F be the distribution function for the inter-arrival times, H be the distribution function for the service times and s the number of servers. These three variables characterize the queueing process formulation completely. A compact notation indicating this characterization is through a string of three symbols – $A/B/C$. A represents the form of F . If it is exponential then the symbol M is used; if Erlangian then the symbol E is used; and if the distribution is general then the symbol G is used. Similarly, B represents the form of H . C represents the number of servers. Thus, $M/M/s$ indicates a queueing process with F and H exponentially distributed and s servers. $X(t)$ has the Markov property only for the $M/M/s$ queue.

6.5 Case Study K [Cont.] (Supermarket Operation)

The system characterization for this problem was done in Chapter 3, Section 6.11. The variable of interest is $N(t)$, the number of people either in the queue or being served at time t . A suitable formulation to use as a dummy in the modelling of this problem is the queueing process formulation discussed in Section 6.4. In this section we develop two models using this approach.

MODEL K.1 (Markov Formulation)

We assume the following:

- (i) The inter-arrival times are statistically independent and identical and from an exponential distribution with parameter λ .
- (ii) The service times are statistically independent and identical and from an exponential distribution with parameter μ .
- (iii) The number of servers is s .
- (iv) Arriving customers join a single queue, and as soon as a server becomes free the server takes the customer at the head of the queue for service.

Let $N(t)$ represent the number of customers either in the queue or being serviced, and $p_n(t)$ be the probability that $N(t) = n$, $n = 0, 1, 2, \dots$. Then we have

$$\sum_{n=0}^{\infty} p_n(t) = 1 \quad (36)$$

Let $t = 0$ correspond to the time the supermarket opens in the morning. We assume that $p_n(0) = 0$ for $n \neq 0$ and $p_0(0) = 1$, implying that there is no customer when the supermarket opens. Whenever $N(t) < s$, one or more of the

servers is idle. The number of idle servers at time t equals zero if $N(t) \geq s$ and equals $s - N(t)$ if $N(t) < s$. All the servers are idle when $N(t) = 0$.

MODEL K.2 (Non-Markov Formulation)

The assumptions regarding the arrival and service times, as well as the queue discipline of the previous model, are very restrictive. We alter these assumptions in this model. More specifically we assume the following:

- (i) At $t = 0$ there are no customers.
- (ii) The first customer arrives at time X_1 and the subsequent customers arrive with inter-arrival times being $X_2, X_3, X_4, \dots$. Thus, the second customer arrives at $t = X_1 + X_2$; the third at $t = X_1 + X_2 + X_3$ and so on. $X_i, i \geq 1$, are independent and identically distributed random variables with distribution function F .
- (iii) The time required to service with the i th customer is $Y_i, Y_i, i \geq 1$, are independent and identically distributed random variables with a distribution function H .
- (iv) There are s servers (numbered 1 through s), and as result there are s separate queues.
- (v) The arriving customer joins the shortest queue.
- (vi) No queue changing is allowed - i.e. once a customer joins a queue no change is allowed. This is justified when there are physical barriers which prevent customers changing queues.

As before $N_i(t) 1 \leq i \leq s$ represents the queue length associated with server i at time t . Server i is idle if $N_i(t) = 0$, and busy otherwise. At time t the total number of people either waiting or being served is $N(t)$, given by:

$$N(t) = \sum_{i=1}^s N_i(t) \quad (37)$$

A slightly more refined formulation is one where customers can change queues. A simple case is one where a customer moves to the adjacent queue if the adjacent queue length becomes smaller than the length of the queue in front of the customer.

6.6 Renewal Process Formulations

In a renewal process formulation the time interval between events is a sequence of independent and identically distributed random variables with a distribution function G . Such a formulation is used extensively in modelling the operation of unreliable components where an event corresponds to a failure and the instantaneous replacement of the failed component by a new one.

6.7 Case Study I [Cont.] (Component Reliability)

The system characterization for this problem was done in Chapter 3, Section 6.9. We employ the same symbols as used in the system characterization and the variable of interest is $N(t)$ - the number of replacements of the element in the interval $[0, t)$ with the element being new at $t = 0$. The elements are identical and the failure time is given by a distribution function G .

MODEL I.1

We assume that the failure is detected the instant it occurs, and that all failed items are replaced by new ones instantaneously. As indicated in the system characterization, this is an idealization which is justified if the time to replace is small in comparison to the mean time to failure. By viewing a failure and replacement as an event, we have events occurring randomly over time. Since the replacement elements are identical (in a statistical sense) the time intervals between events correspond to failure times which form a sequence of independent and identically distributed random variables with distribution function G . This is best modelled by a renewal process formulation which takes the following form when applied to this problem.

Let T be the time interval of interest and $N(T)$ be the number of replacements carried out. To find the number of replacement elements needed it is necessary to obtain the statistical characterization of $N(T)$, for example the distribution function or its moments. Alternatively, if there are n spares and we wish to find the time τ that these will keep the machine operational, the problem reduces to finding the statistical characterization of τ .

MODEL I.2

Suppose that there are no spares and that the failed element can be repaired, making the machine operable once more. If we assume that the failure distribution of a repaired element is nearly the same as that for the new element, we have a repair which is called "back to new". If the time to repair is random, then the variable characterizing the system can be specified as $X(t)$ with

$$\begin{aligned} X(t) &= 1 \text{ if element is working} \\ &= 0 \text{ if failed} \end{aligned} \quad (38)$$

Let H represent the distribution function characterizing the time to repair, and G represent the distribution function for the time to failure. Then, in this case, $X(t)$ can be modelled by a semi-Markov process formulation discussed in Section 6.1 with two states. More specifically, we have:

$$(i) \quad s_1 = 1, s_2 = 0 \quad (39)$$

$$(ii) \quad Q = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad (40)$$

and

$$(iii) G_{12}(t) = F(t) \quad \text{and} \quad G_{21}(t) = H(t) \quad (41)$$

If $H(t) = U(t - \rho)$, with $U(y) = 0$ for $y < 0$ and $U(y) = 1$ for $y \geq 0$, then it implies a constant repair time ρ .

7 Continuous State/Discrete Time Formulations

The variables of the formulation assume a continuous range of values, and are characterized for discrete values of the independent time variable t . Without loss of generality we can assume that the discrete values of t correspond to the set of natural integers. Thus, the variables are of the form $X_i (\equiv X(t = t_i, \omega))$.

7.1 General Formulation

A fairly general formulation is one where X_i satisfies an equation

$$X_{i+1} = g(X_i, X_{i-1}, \dots, X_{i-n}; u_i, u_{i-1}, \dots, u_{i-m}; W_i, W_{i-1}, \dots, W_{i-k}, \theta_i) \quad (42)$$

where $\{u_i\}$ is a specified sequence, $\{W_i\}$ is an unknown sequence of independent random variables; θ_i is a set of parameters which can change with time, as the subscript corresponds to the independent variable time t .

Assume that $X_j, -\infty < j \leq i$ is known. The evolution of $X_j, j > i$ is uncertain due to the unknown random sequence $\{W_j\}$. Note that if the random sequence $\{W_j\}$ is identically zero (i.e. there is no uncertainty) then (42) reduces to the difference equation formulation of the form studied in Section 4 of Chapter 5. Thus, we can view (42) as a stochastic counterpart of the deterministic difference equation formulation.

The sequence $\{X_i\}$ generated by (42) does not have the Markov property as X_{i+1} depends not only on X_i but also on $X_{i-j}, j > 0$.

7.2 Markov Formulation

If n, m and k in (42) are equal to zero, then we have

$$X_{i+1} = g(X_i, u_i, W_i, \theta_i) \quad (43)$$

and in this case the sequence $\{X_i\}$ has the Markov property.

The general formulation given by (42) can be transformed into a formulation having the Markov property by an enlarged state space, i.e. by defining a variable Z_i which is related to the sequence $\{X_i\}$, $\{u_i\}$ and $\{W_i\}$ in a manner similar to that in Section 4.2 of Chapter 5. The dimension of Z_i would depend on n, m and k .

7.3 Time Series Formulation

There is a class of formulations in which X_i is the sum of two components - Y_i which changes in a deterministic manner and V_i which changes in an uncertain

manner, i.e.:

$$X_i = Y_i + V_i \quad (44)$$

The changes in V_i are given by a linear difference equation formulation of the form

$$V_i = \sum_{j=1}^n \alpha_j V_{i-j} + \sum_{j=1}^m \beta_j W_{i-j} \quad (45)$$

where $\{W_i\}$ is a sequence of independent and identically distributed Gaussian random variables with zero mean and variance σ^2 . The parameters $(\alpha_j, 1 \leq j \leq n$ and $\beta_j, 1 \leq j \leq m)$ are constrained so that the sequence $\{V_i\}$ is stationary. The constraints which ensure this are that the roots of $P(\delta) = 0$ and $Q(\delta) = 0$ lie inside the unit circle, where

$$P(\delta) = \delta^n - \sum_{j=1}^n \alpha_j \delta^{n-j} \quad \text{and} \quad Q(\delta) = \sum_{j=1}^m \beta_j \delta^{m-j} \quad (46)$$

The difference equation formulation for V_i is called an autoregressive moving average (ARMA) formulation of order n and m . When $m = 1$ it is called an autoregressive (AR) formulation.

7.4 Case Study L [Cont.] (Demand for Soft Drinks)

The system characterization for this problem was done in Chapter 3, Section 6.12. The variable of interest is X_t , the demand for the soft drink in period t . In this section we build a model for the simplest characterization, where the system is viewed as a "black box" with one variable X_t . The period is a month, and X_t represents the monthly demand.

MODEL L.1

We assume that X_t consists of a deterministic component D_t and a stochastic component V_t .

The deterministic component D_t is assumed to be made up of two components: g_t , which represents growth (due to population increase) and s_t , which represents seasonal variations (e.g. extra demand during summer months). We assume that

$$g_t = a + bt \quad (47)$$

and that

$$s_t = s_{t-12} \quad (48)$$

Thus, we have

$$X_t = a + bt + s_t + V_t$$

From (47) we have the following:

$$(i) \quad l_t = g_t - g_{t-1} = (1 - \Delta)g_t = b \quad (49)$$

where Δ is the backward shift operator; i.e. $\Delta g_t = g_{t-1}$, and

$$(ii) \quad m_t = l_t - l_{t-1} = (1 - \Delta)l_t = (1 - \Delta)^2 g_t = 0 \quad (50)$$

i.e. by differencing, the effect of growth is removed.

From (48) we have the following:

$$r_t = s_t - s_{t-12} = (1 - \Delta^{12})s_t = 0 \quad (51)$$

i.e. by taking the difference with a lag of 12 (i.e. Δ^{12}) the effect of seasonal variation is removed.

Thus, defining a sequence Y_t as follows:

$$Y_t = (1 - \Delta)^2 (1 - \Delta^{12})X_t \quad (52)$$

we have removed the effect of growth and seasonal variation and are left only with the stochastic part. This we model by a ARMA formulation of order n and m , i.e. Y_t is modelled by

$$Y_t = \sum_{j=1}^n a_j Y_{t-j} + \sum_{j=1}^m \beta_j W_{t-j} \quad (53)$$

Once the order n and m and the parameters are estimated using the data, estimates of future values of Y_t can be obtained from (53) by assuming W_t to be zero; this in turn yields the future values of X_t from (52).

Note that we need not carry out the first differencing twice. The differencing of (49) leaves a constant b and the effect of this is removed by the differencing of (51). Thus, Y_t defined by

$$Y_t = (1 - \Delta)(1 - \Delta^{12})X_t \quad (54)$$

is the more appropriate sequence to be modelled by (53) as opposed to Y_t generated by (52).

8 Continuous State/Continuous Time Formulations

The variables of this formulation are of the form $X(t) (\equiv X(t, \omega))$ with both the variable X and the independent time variable t assuming a continuous range of values. The formulations can be divided into three types based on the nature of changes in $X(t)$:

- Type A:* The time history of $X(t)$ is a continuous function of t with no jumps.
- Type B:* The time history of $X(t)$ is a function with jumps at random time instants and in between jumps the function does not change.
- Type C:* The time history of $X(t)$ is not only a continuously changing function of t but also undergoes jumps at random time instants.

Thus in the case of Type B there is an underlying point process which affects the variable $X(t)$, whereas in Type A, $X(t)$ is affected by a process which changes continuously over time. Type C is a combination of both.

The two well-known formulations are the Poisson process (Type B) and the Wiener process (Type A). A variety of continuous state/continuous time formulations have been developed using these as the building blocks. We give a brief presentation of these two basic processes and then discuss two other formulations.

8.1 Poisson Process

This type of process was briefly discussed in Section 6.3. Let $N(t)$ represent the count of events, occurring randomly over time, in the interval $[0, t)$ and let $N(0) = 0$. $N(t)$ is a stationary Poisson process if the distribution of $N(t)$ is given by a Poisson distribution function, i.e.:

$$\text{prob}\{N(t) = k\} = \{(\lambda t)^k e^{-\lambda t}\} / k! \quad (55)$$

for $k = 0, 1, 2, \dots$. Two extensions of this process are: the non-stationary Poisson process and the doubly stochastic Poisson process.

8.2 Wiener Process

The Wiener process, $W(t)$, is a continuous process which changes erratically and has many unusual properties, some of which are listed below:

- (i) $W(t)$ has zero mean; i.e. $E\{W(t)\} = 0$.
- (ii) $W(t)$ has independent increments; i.e. for $t_1 < t_2 < t_3 < t_4$
 $E\{[W(t_2) - W(t_1)][W(t_4) - W(t_3)]\} = 0$.
- (iii) $W(t)$ has the Markov property.
- (iv) $E\{W(t)W(t')\} = \min(t, t')$.
- (v) $W(t)$ has a Gaussian distribution.
- (vi) $W(t)$ is continuous in t but is non-differentiable.

8.3 Compound Poisson Process Formulation

This involves a Poisson process $N(t)$ and a sequence Z_i , $i \geq 1$, of independent and identically distributed random variables from a distribution function G . The process $X(t)$ is given by

$$X(t) = \sum_{i=1}^{N(t)} Z_i \quad (56)$$

$X(t)$ can be viewed as a sum of random variables and changing at discrete time instants which correspond to events of a Poisson process. Alternatively, we can view Z_i as a mark attached to event i and $X(t)$ as the cumulative sum of

marks associated with the events over the interval $[0, t]$. We illustrate the use of this formulation as a dummy in modelling the following two case studies.

8.4 Case Study I [Cont.] (Component Reliability)

The system characterization for this problem was done in Chapter 3, Section 6.9. Two models for component failure using the "black-box" approach (Models I.1 and I.2) were developed in Section 6.7. In this section we build a model for component failure due to crack propagation.

MODEL I.3

We assume that the component fails when the crack length reaches a critical length L . The crack propagation is due to shocks which occur according to a Poisson process with parameter λ . The damage caused by each shock is non-negative and assumed to be random and statistically independent. In other words, the increase in crack length with shock i is an independent random variable, X_i , with a distribution function G . Let t be the age of the component and $Y(t)$ be the crack length by age t . Then we have

$$Y(t) = \sum_{i=1}^{N(t)} X_i \quad (57)$$

where $N(t)$ is the number of shocks received by the component by age t . Let the time to failure be denoted by τ . Then τ is a random variable with a distribution function F given by

$$\bar{F}(t) = 1 - F(t) = \text{prob}\{\tau > t\} = \text{prob}\{Y(t) < L\} \quad (58)$$

Thus, the model uses a compound Poisson process as a dummy. Using the failure distribution F (obtained from (58)) in Model I.1 we can obtain the solution to the problem.

8.5 Case Study J [Cont.] (Speed of Aeroplanes)

The system characterization for this problem was done in Chapter 3, Section 6.10. In Section 4.4 of this chapter we discussed three models involving regression formulations as dummies. In this section we discuss a model which uses a compound Poisson process formulation as a dummy.

MODEL J.4

As described in the system characterization, the changes to the maximum speed occur due to technological breakthroughs. Let $t = 0$ correspond to the year 1900. We assume that the breakthroughs occur according to a Poisson process with parameter λ . This implies that the time between breakthroughs is

exponentially distributed with mean $(1/\lambda)$. We assume that the increase in speed due to the i th breakthrough, Y_i , is a random variable with a distribution G , and that the increases are statistically independent. In this case the maximum speed achieved at time t is given by

$$X(t) = \sum_{i=1}^{N(t)} Y_i \quad (59)$$

if $N(t)$ is the number of breakthroughs in the interval $[0, t]$.

8.6 Differential Equation Formulations

A fairly general Markov process formulation is given by a differential equation formulation of the form:

$$dX(t) = f_1(X(t))dt + f_2(X(t))dW(t) + f_3(X(t))dN(t) \quad (60)$$

where $W(t)$ is a Wiener process and $N(t)$ is a Poisson process. The initial condition $X(0)$ can be random and needs to be specified probabilistically. The functions f_1 , f_2 and f_3 must be constrained to ensure the existence of the solution (in a stochastic sense).

The differential equation is linear if the functions f_1 , f_2 and f_3 are linear in their arguments; if not, it is a non-linear differential equation. The above formulation can be viewed as the stochastic counterpart of the deterministic ordinary differential equations formulations studied in Chapter 5, Section 5.

Note that in the formulation given by (60) we have $X(t)$ changing continuously due to the first two terms on the right-hand side of the equation and undergoing jumps due to the last term. Thus $X(t)$ is of Type C.

Notes and References

Our presentation has been very terse and introductory. There are many excellent textbooks which cover a range of stochastic formulations and their applications; [1]–[8] are a small sample.

Regression formulations have been used extensively in the modelling of economic systems. Further details of this type of formulation can be found in [9]–[11] or in any book on econometrics (e.g. [12] and [13]).

There are a large number of books dealing with specific stochastic formulations and their applications. We give a small list: [14] and [15] deal with Markov chains; [16]–[18] deal with time-series formulations; [19]–[21] deal with point processes, with the last reference a collection of papers dealing with both theory and applications, and [22]–[24] deal with queues.

A proper study of continuous time Markov processes requires a rigorous approach. A classic book in this mould is [25], and since then a large number of books have appeared on this topic (e.g. [26] and [27]). For more on stochastic differential equations, see [28]–[31].

We have not discussed many other types of stochastic formulations – for example, random integral equations [32]; branching processes [33]; random fields [34]; and storage processes [35], to name a few.

There are a large number books on the application of stochastic formulations to modelling problems from specific disciplines: [36]–[45] are a small sample.

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Analysis of Mathematical Formulations – II

1 Introduction

In Chapter 6 we discussed the analysis of the underlying mathematical formulations used in models of deterministic systems and examined the variety of techniques available. The techniques of analysis for stochastic formulations are different from those for deterministic formulations. In this chapter we examine techniques of analysis for the stochastic formulations discussed in Chapter 7. As indicated in Chapter 7, stochastic formulations belong to the theory of stochastic processes. As such we start with a brief general discussion on the analysis of stochastic processes. Following this we discuss techniques of analysis for some specific stochastic formulations.

2 Analysis of Stochastic Processes

Let $X(t) (\equiv X(t, \omega))$ be the variable of the stochastic process which evolves with t according to the underlying mathematical formulation defining the process $X(t)$. In this section we first discuss different types of analysis and later we discuss two different approaches to analysis.

2.1 Probability Distribution Function

An important problem in analysis of stochastic processes is to obtain the joint distribution function $F(x_1, t_1; x_2, t_2; \dots; x_n, t_n)$ given by

$$F(x_1, t_1; x_2, t_2; \dots; x_n, t_n) = \text{prob} \{X(t_1) \leq x_1; X(t_2) \leq x_2; \dots; X(t_n) \leq x_n\} \quad (1)$$

for arbitrary n . If the process has the Markov property we need to obtain the distribution function for $n = 2$; i.e. $F(x_1, t_1; x_2, t_2)$ for arbitrary x_1, x_2 and t_1, t_2 . From this, the joint distribution function (1) can be obtained using conditional argument as indicated in Section 2.1 of Chapter 7.

2.2 Moment Analysis

The joint distribution function completely characterizes the probabilistic evolution of $X(t)$ with t . Often one is content with only moment characterization. Let $M_j(t)$ represent the j th moment of $X(t)$, given by

$$M_j(t) = E[X^j(t)]; \quad j = 1, 2, \dots \quad (2)$$

In particular, the first moment $M_1(t)$ and the variance $\sigma^2(t)$ are of special interest. The variance $\sigma^2(t)$ is related to the first two moments as follows:

$$\sigma^2(t) = M_2(t) - M_1^2(t) \quad (3)$$

$M_1(t)$ characterizes the mean of $X(t)$, and the variance $\sigma^2(t)$ characterizes the dispersion in $X(t)$ about the mean.

$M_j(t)$, as defined by (2), does not incorporate the relationship between $X(t)$ and $X(\tau)$ for $\tau \neq t$. Moments which incorporate this aspect are given by

$$C_{jk}(t, \tau) = E\{[X(t) - M_1(t)]^j [X(\tau) - M_1(\tau)]^k\} \quad (4)$$

$1 \leq j, k < \infty$. When $j = k = 1$, $C_{11}(t, \tau)$ is called the covariance function and it characterizes the statistical correlation between $X(t)$ and $X(\tau)$. In the case of a stationary stochastic process, we have

$$C_{jk}(t, \tau) = C_{jk}(t - \tau) \quad (5)$$

2.3 Steady State Analysis

In steady state analysis one is interested in the analysis of the process as $t \rightarrow \infty$. If the process is stable, then as $t \rightarrow \infty$, $X(t)$ reaches steady state and the distribution function characterizing $X(t)$ becomes independent of t , i.e.

$$F(x, t) \rightarrow F(x) \quad (6)$$

As a consequence

$$M_j(t) \rightarrow M_j \quad (7)$$

where M_j , $1 \leq j < \infty$, are constants. In general, it is much simpler to obtain M_j than $M_j(t)$.

2.4 Analysis of Associated Variable

Often the variable of interest is not $X(t)$ itself, but some other variable Y (or $Y(t)$) which is related to $X(t')$ $0 \leq t' \leq t$. We shall call such a variable an associated variable. Such variables are important in many contexts, as will be illustrated through case studies later.

In cases where $X(t)$ assumes only discrete states ($s_1 s_2 \dots s_n$) examples of associated variables are:

- (i) the number of visits to a state s_i in a specified time period starting from some specified initial state;
- (ii) the time taken for the process to return to its starting state for the j th time ($j \geq 1$); and
- (iii) the number of times the process visits two states in succession in a specified time period.

In the case where $X(t)$ assumes a continuous range of values ($-\infty < X(t) < \infty$), examples of associated variables are:

- (i) the number of sign reversals in a specified time period;
- (ii) the fraction of the time for which $X(t)$ exceeds a value b in a specified time interval; and
- (iii) the first time $X(t)$ becomes zero or crosses some level b .

Sometimes it is possible to obtain a complete probabilistic characterization of an associated variable. When this is not possible, one resorts to analysis through moments.

2.5 Two Approaches to Analysis

Two approaches to analysis of stochastic process formulations are analytical and simulation.

In the analytical approach the distribution function, or the moments, of $X(t)$ (or an associated variable $Y(t)$) are obtained using analytical techniques. Often it involves solving either difference, or differential, equations (ordinary or partial). Only for a small class of formulations can these equations be solved in closed form. When this is not possible a computational scheme must be employed. A variety of techniques have been found to be useful in the analytical approach. In particular, Laplace transforms and moment-generating functions have proved to be extremely useful for a wide range of formulations.

When it is difficult to obtain exact analytical solutions one can resort to obtaining analytical expressions for lower and upper bounds to the variables of interest. For a variety of formulations such bounds can be obtained with considerably less effort than that required for the exact solution.

In the simulation approach the stochastic process is simulated on a computer to generate individual time histories (also called realizations) of the process. By repeating the simulation a large number of times, sufficient statistical information about the process is obtained to yield estimates of either the distribution functions (or the moments) of the variables of interest. As such this approach can be viewed as computer experimentation.

In this chapter we will confine our attention to the analytical approach. The simulation approach will be discussed in Chapter 9.

3 Static Formulations

In Section 4 of Chapter 7 we discussed two types of static formulations - analysis of variance and regression. The analysis of variance formulations will be discussed in Chapter 11, and in this section we discuss briefly the analysis of regression formulation.

3.1 Regression Formulations

The structure of such formulations is given by the relationship

$$Y_i = g(X_{1i}, \dots, X_{ni}; \theta) + V_i \quad (8)$$

where $X_{ji} (1 \leq j \leq n, i \geq 1)$ are known variables and $V_i (i \geq 1)$ are unknown random variables with zero mean. An important problem in analysis of such formulations is to obtain the probabilistic characterization of $Y_{i+l} (l > 0)$ given $Y_k (1 \leq k \leq i)$ and $X_{jk} (1 \leq j \leq n; 1 \leq k \leq i+l)$.

If $V_i (i \geq 1)$ is a sequence of uncorrelated random variables, then

$$\begin{aligned} \text{prob} \{ Y_{i+l} \leq y_{i+l} | Y_k = y_k, 1 \leq k \leq i; X_{jk}, 1 \leq j \leq n, 1 \leq k \leq i+l \} \\ = \text{prob} \{ Y_{i+l} \leq y_{i+l} | X_{j(i+l)}, 1 \leq j \leq n \} \end{aligned} \quad (9)$$

As a result, we have:

$$E\{Y_{i+l}\} = g(X_{1(i+l)}, \dots, X_{n(i+l)}; \theta) \quad (10)$$

and

$$\text{var} \{ Y_{i+l} \} = \text{var} \{ V_{i+l} \} \quad (11)$$

However, if $V_i (i \geq 1)$ is a correlated sequence, then (9) is no longer true. The characterization of Y_{i+l} will depend on the nature of the correlation between V_i and $V_j (i \neq j)$. We shall discuss this aspect later when dealing with the analysis of discrete time/continuous state formulations.

3.2 Case Study J [Cont.] (Speed of Aeroplanes)

In Section 4.4 of Chapter 7 we formulated three models (Models J.1 to J.3) involving regression formulations for predicting the maximum speed of aeroplanes. In this section we consider the analysis of Model J.3.

MODEL J.3

The maximum speed achieved by time t is a random variable $X(t)$ given by equations (18)–(20) of Chapter 7. Since the uncertainty in $X(t)$ is solely due to $V(t)$, an uncorrelated random sequence with zero mean and variance σ^2 , we

have the $E[X(t)]$ and the $\text{var}[X(t)]$ given by

$$E[X(t)] = \begin{cases} c_1 + d_1(t - 1900), & 1900 \leq t \leq 1940 \\ c_2 + d_2(t - 1940), & 1940 \leq t \leq 1980 \\ c_3 + d_3(t - 1980), & 1980 \leq t \leq 2020 \end{cases} \quad (12)$$

and

$$\text{var}[X(t)] = \sigma^2, \quad 1900 \leq t \leq 2020 \quad (13)$$

In other words, the mean is given by a function which is piecewise linear and the variance is constant.

4 Discrete State/Discrete Time Formulations

In Section 5 of Chapter 7 we discussed discrete state/discrete time formulations where the discrete states assumed by X_t are denoted by $s_1, s_2, \dots, s_r$ and the time variable t assuming integer values. In particular, if X_t has the Markov property, then the formulation is specified by an $r \times r$ one-step transition matrix $P(t)$:

$$P(t) = \begin{bmatrix} P_{11}(t) & \dots & P_{1r}(t) \\ P_{r1}(t) & \dots & P_{rr}(t) \end{bmatrix} \quad (14)$$

where

$$P_{jk}(t) = \text{prob}\{X_{t+1} = s_k | X_t = s_j\}$$

for $1 \leq j, k \leq r$. The elements of the matrix are subject to the constraints given by equation (24) of Chapter 7.

The initial state X_0 is specified through an r -dimensional probability vector $p(0)$ with

$$p_i(0) = \text{prob}\{X_0 = s_i\}, \quad 1 \leq i \leq r \quad (15)$$

and the elements of $p(0)$ subject to the constraint given by equation (27) of Chapter 7. In this section we discuss some aspects of the analysis of such formulations. We confine our attention to the case where r is finite.

4.1 Evolution of X_t

Let $p(t)$ be an r -dimensional vector with

$$p^T(t) = [p_1(t), \dots, p_r(t)] \quad (16)$$

which characterizes the evolution of X_t , i.e.:

$$p_i(t) = \text{prob}\{X_t = s_i\}, \quad 1 \leq i \leq r \quad (17)$$

Then, we have

$$p^T(t+1) = P(t)p^T(t) \quad (18)$$

for $t \geq 0$. Using the initial probability vector $p(0)$ as the initial condition, the above equation can be solved recursively to obtain $p(t)$ for $t \geq 0$. Note that

$p(t+1)$ can also be rewritten as

$$p^T(t+1) = \tilde{P}(t, t')p^T(t') \quad (19)$$

for $0 \leq t' \leq t$, with $\tilde{P}(t, t')$ given by the relation

$$\tilde{P}(t, t') = \prod_{j=t'}^t P(j). \quad (20)$$

$\tilde{P}(t, t')$ can be viewed as a $(t+1-t')$ -step transition matrix which characterizes the transition from time t' to time $(t+1)$. When the chain is stationary, i.e. $P(t) = P$ for all t , then

$$\tilde{P}(t, t') = P^{(t-t')} \quad (21)$$

4.2 Steady State Probabilities

The steady state behaviour of X_t , i.e. the behaviour of X_t as $t \rightarrow \infty$, for the case where the chain is stationary, depends on the structure of the one-step transition matrix P .

In this context the decomposition of the states into transient and recurrent plays an important role. A state i is said to be transient (recurrent) if the probability of the process not eventually returning to the state is non-zero (zero). The recurrent states can be grouped into different equivalence classes with the states belonging to an equivalence class being accessible to each other. If there be no transient states and the recurrent states belong to one single equivalence class, then the chain is said to be irreducible; if not it is called a reducible chain.

For an irreducible stationary Markov chain, as $t \rightarrow \infty$, $p(t) \rightarrow p^*$, a steady state vector which satisfies the following relationships

$$p^* = P^T p^* \quad (22)$$

with the elements of p^* summing to one, i.e.

$$\sum_{i=1}^r p_i^* = 1 \quad (23)$$

The steady state analysis for a reducible chain is more involved.

4.3 Analysis of an Associated Variable

We shall confine our discussion to a study of an associated variable called "occupation time". This variable refers to the number of times the process X_t occupies a certain state in a given time period.

Let $N_{ij}^{(n)}$ be the number of times X_t visits state s_j in a time interval n , given that initially it was in state s_i . If the chain is stationary and irreducible, then we have the following asymptotic result - i.e.:

$$\lim_{n \rightarrow \infty} N_{ij}^{(n)}/n \rightarrow p_j^* \quad (24)$$

where p_j^* is the j th component of p^* given by (22) and (23). Note that the initial starting state has no effect on this probability.

4.4 Case Study G [Cont.] (Weather Changes)

In Section 5.3 of Chapter 7 we formulated three different models (Models G.1 to G.3) for modelling weather changes. In this section we carry out an analysis of Model G.1.

MODEL G.1

Since there are only three states (states 1, 2 and 3 corresponding to sunny, partly sunny and cloudy weather), the one-step transition matrix is given by a 3×3 matrix:

$$P = \begin{bmatrix} P_{11} & P_{12} & 1 - P_{11} - P_{12} \\ P_{21} & P_{22} & 1 - P_{21} - P_{22} \\ P_{31} & P_{32} & 1 - P_{31} - P_{32} \end{bmatrix} \quad (25)$$

with p_{ij} ($1 \leq i \leq 3, 1 \leq j \leq 2$) being non-negative variables constrained such that the last entry in each row is also non-negative. Note that, in the way we have written the matrix, each row sums to unity.

Since the weather can change arbitrarily from one state (i.e. sunny, partly sunny or cloudy) to any other, the assumption that the chain is irreducible is justified. Our interest is to obtain the expected number of sunny and partly sunny days in a year. This corresponds to obtaining the expected number of visits to states 1 and 2 respectively over a year. As there are 365 days in a year, and since this is a large number, we can use the asymptotic results of Section 4.3 to yield:

$$\begin{aligned} E \{\text{sunny days in a year}\} &\sim 365 p_1^* \\ E \{\text{partly sunny days in a year}\} &\sim 365 p_2^* \end{aligned} \quad (26)$$

p_1^* and p_2^* are given by:

$$\begin{aligned} (1 - P_{12})p_1^* + (1 - P_{11})p_2^* &= (1 - P_{11} - P_{12}) \\ (1 - P_{22})p_1^* + (1 - P_{21})p_2^* &= (1 - P_{21} - P_{22}). \end{aligned} \quad (27)$$

(Note (27) is obtained using (25) in (22).)

5 Queueing Process Formulations

In the queueing process formulation the variable $X(t)$ represents the number of customers, either being served or waiting to be served, at time t . In Section 6.4 of Chapter 7 we discussed the underlying structure of the queueing process and defined four different types of queues – $M/M/S$, $M/G/S$, $G/M/S$ and $G/G/S$, respectively. In this section we discuss the analysis of some of these processes.

5.1 Evolution of $X(t)$

In the case of the $M/M/S$ queue, $X(t)$ has the Markov property. As such it is not too difficult to obtain the probabilistic characterization of $X(t)$ as it evolves over t . As will be shown later, this probabilistic characterization can be obtained as the solution of a set of coupled linear ordinary differential equations. The steady state probabilities, if they exist, can also be obtained fairly easily.

In the case of $M/G/S$ or $G/M/S$ or $G/G/S$ queues, $X(t)$ no longer has the Markov property; as a result the analysis of such formulation is more difficult. We shall briefly discuss the analysis of the $G/M/S$ queue as an example of this class of problems.

For the $G/M/S$ queue one can use essentially two different approaches. In both the analysis is reduced to a study of a formulation having the Markov property. In the first approach we define a variable $Y(t)$ which represents the time that has elapsed since the last arrival. $Y(t)$ is a sawtooth function increasing linearly with t and becoming zero with the arrival of each customer. A vector $Z(t)$, defined thus:

$$Z(t) = \{X(t), Y(t)\}^T \quad (28)$$

can be shown to have the Markov property, and hence is easier to analyse than $X(t)$. In the second approach the queue is studied in terms of $X(t)$ only at time instants at which a customer arrives. Let X_n represent $X(t)$ at the time instant of the arrival of the n th customer. Then it can be shown that the sequence X_n , $n \geq 1$, has the Markov property. More specifically, X_n can be viewed as a Markov chain with the states being the set of non-negative integers.

5.2 Case Study K [Cont.] (Supermarket Operation)

In Section 6.5 of Chapter 7 we discussed two models (Models K.1 and K.2) involving queueing process formulation for modelling the operation of a supermarket checkout counter. Model K.1 involved a $M/M/S$ queue formulation, whilst Model K.2 involved a $G/G/S$ queue formulation. In this section we carry out an analysis of Model K.1.

MODEL K.1

The characterization of customer arrival and service and the queue discipline are given by assumptions (i)–(iv) of Model K.1 in Section 6.5 of Chapter 7.

Let $N(t)$ represent the number of customers either in the queue or being served at time t . $N(t)$ is a random variable which can assume only non-negative integer values. $N(t) = 0$ corresponds to all the servers being idle and $N(t) \geq s$ corresponds to all the servers being busy at time t . Let $p_n(t)$ be the probability

that $N(t) = n, n = 0, 1, 2, \dots$; then we have

$$\sum_{n=0}^{\infty} p_n(t) = 1 \quad (29)$$

Let $N(t) = n$. Then at time $t + \delta t$ either there is no change in $N(t)$ or it can either increase or decrease (provided $N(t) \neq 0$). Because of the inter-arrival and service times being exponential we have, conditional on $N(t) = n$:

$$N(t + \delta t) = \begin{cases} n+1 & \text{with probability } \lambda \delta t + o(\delta t) \\ n & \text{with probability } (1 - \lambda \delta t - \mu_n \delta t) + o(\delta t) \\ n-1 & \text{with probability } \mu_n \delta t + o(\delta t) \end{cases} \quad (30)$$

$N(t)$ changing by two or more in δt is $o(\delta t)$ and can be ignored as $\delta t \rightarrow 0$.

Since there are s servers operating in parallel the variable μ_n is given by:

$$\begin{aligned} \mu_n &= s\mu \text{ for } n \geq s \\ &= n\mu \text{ for } n \leq s \end{aligned} \quad (31)$$

As a result we have for $n > 0$:

$$p_n(t + \delta t) = \text{prob}\{N(t + \delta t) = n\} = p_{n-1}(t)\{\lambda \delta t\} + p_n(t)\{1 - \lambda \delta t - \mu_n \delta t\} + p_{n+1}(t)\{\mu_{n+1} \delta t\} + o(\delta t). \quad (32)$$

We have used the conditional argument in obtaining (32) where the first term corresponds to $N(t) = n - 1$ with one arrival and no departure, the second term to $N(t) = n$ with no arrival or departure and the third term to $N(t) = n + 1$ with one departure and no arrival. Taking the limit, we have:

$$p'_n(t) = dp_n(t)/dt = -(\lambda + \mu_n)p_n(t) + \lambda p_{n-1}(t) + \mu_{n+1}p_{n+1}(t) \quad (33)$$

Similarly, we have for $N(t) = 0$:

$$p'_0(t) = dp_0(t)/dt = -\lambda p_0(t) + \mu_1 p_1(t). \quad (34)$$

We assume that $t = 0$ corresponds to the instant the supermarket opens in the morning. Since there are no customers before the supermarket opens, we have:

$$p_n(0) = 0 \text{ for } n \neq 0 \quad (35)$$

and

$$p_0(0) = 1$$

These define the initial conditions for (33) and (34).

STEADY STATE PROBABILITIES

Under certain conditions, for large t , $p_n(t)$, $n \geq 0$, approach steady state values p_n^* which are independent of t . More specifically:

$$p_n(t) \rightarrow p_n^* \text{ as } t \rightarrow \infty \quad (36)$$

These can be obtained from (33) and (34) by setting the derivatives to zero and solving the resulting system of linear algebraic equations. It can be shown (after some algebraic manipulation) that

$$p_0^* = \left\{ \sum_{r=0}^s \frac{(s\rho)^r}{r!} + \frac{\rho^{s+1}s^s(1-\rho)^{-1}}{s!} \right\}^{-1} \quad (37)$$

and

$$p_n^* = \begin{cases} (s\rho)^n p_0^*/n! & \text{for } n \leq s \\ s^s \rho^s p_0^*/s! & \text{for } n \geq s \end{cases} \quad (38)$$

where $\rho = \lambda/s\mu$. Note that the condition for the existence of this limiting distribution is given by

$$\rho = \lambda/s\mu < 1 \quad (39)$$

EXPECTED QUEUE LENGTH

Under steady state conditions (i.e. the process has been operating for a long time and that (39) is satisfied) let QL represent the number of people waiting in the line and L the expected value of it. Then, we have

$$L = E[QL] = \sum_{n=s+1}^{\infty} (n-s)p_n^* \quad (40)$$

for there is a queue only when the number of customers exceeds s . Using p_n^* from (37) and (38) we have

$$L = \rho p_s^*/(1-\rho)^2 \quad (41)$$

indicating that the average queue length increases to infinity as $\rho \rightarrow 1$.

WAITING TIME FOR A CUSTOMER

Let the waiting time for a customer under steady state conditions be denoted by W and let

$$F(x) = \text{prob}\{W \leq x\} \quad (42)$$

Since there is no waiting if the number of customers is less than or equal to s , we have

$$\begin{aligned} F(0) &= \text{prob}\{N(t) \leq s\} \\ &= p_0^* \sum_{n=0}^{s-1} (s\rho)^n/n! \end{aligned} \quad (43)$$

When the number of customers $N(t) = n$ and n is greater than s , then there are $(n-s)$ waiting to be served, and in this case we have

$$\begin{aligned} \text{prob}\{x < W \leq x + \delta x | N(t) = n\} \\ = \frac{e^{-s\mu x} (s\mu x)^{n-s}}{n-s} (s\mu) \delta x \end{aligned} \quad (44)$$

This follows, as W is the sum of the service times for $(n-s)$ customers with s servers. Since the service times are exponential the server has a gamma density function as indicated above. Since:

$$\text{prob}\{N(t) = n\} = p_n^* \quad (45)$$

we have

$$dF(x) = \sum_{n=s}^{\infty} p_n^* \frac{e^{-s\mu x} (s\mu x)^{n-s}}{(n-s)!} (s\mu) dx \quad (46)$$

which on simplification gets reduced to

$$dF(x) = s\mu p_s^* e^{-(s\mu - \lambda)x} dx \quad (46')$$

From (43) and (46') we have the expected waiting time for a customer given by

$$E[W] = \int_0^{\infty} x dF(x) = p_s^* / [s\mu(1 - \rho)^2] \quad (47)$$

again indicating that the expected waiting time increases to infinity as $\rho \rightarrow 1$.

6 Renewal Process Formulations

As indicated in Section 6.6 of Chapter 7, the renewal process is a special type of a point process where the time interval between events is a sequence of independent and identically distributed random variables with a distribution function $G(x)$. In this section we discuss the analysis of renewal process under the assumption that the origin $t = 0$ is a renewal point. When $t = 0$ is not a renewal point then the analysis is more complicated.

Let $N(t)$ represent the number of renewals in the interval $[0, t]$ and let X_i represent the time between the $(i-1)$ st and the i th renewal. We treat the renewal at the origin $t = 0$ as the zero-th renewal.

6.1 Analysis of $N(t)$

The crucial step in the analysis is the following statement:

$$N(t) \geq n \text{ if and only if } S_n \leq t \quad (48)$$

where S_n is defined as follows:

$$S_n = \sum_{i=1}^n X_i \quad (49)$$

Since S_n is the sum of n independent and identically distributed random variables, the distribution function $H_n(x)$ of S_n is the n -fold convolution of $G(x)$ with itself.

From (48) we have

$$\begin{aligned} p_n(t) &= \text{prob}\{N(t) = n\} \\ &= \text{prob}\{N(t) \geq n\} - \text{prob}\{N(t) \geq n+1\} \\ &= \text{prob}\{S_n \leq t\} - \text{prob}\{S_{n+1} \leq t\} \\ &= H_n(t) - H_{n+1}(t) \end{aligned} \quad (50)$$

6.2 Expected Number of Renewals

Let $M(t)$ represent the expected number of renewals in $[0, t]$, i.e.:

$$M(t) = E[N(t)] \quad (51)$$

One way of obtaining $M(t)$ is by using the relationship

$$M(t) = \sum_{n=0}^{\infty} n p_n(t) \quad (52)$$

An alternative approach is via the conditional argument based on the observation that the renewal process repeats itself after each renewal. Let the first renewal occur at $X_1 = x$. Then conditioned on this, we have

$$M(t|X_1 = x) = \begin{cases} 0 & \text{if } x \geq t \\ M(t-x) + 1 & \text{if } x < t \end{cases} \quad (53)$$

By removing the conditioning, i.e.

$$M(t) = \int_0^{\infty} M(t|X_1 = x) dG(x) \quad (54)$$

we have the result

$$M(t) = G(t) + \int_0^t M(t-x) dG(x) \quad (55)$$

This is a linear integral equation which can be solved analytically for simple forms for $G(x)$. In general, one would need a computational technique to obtain $M(t)$ from (55).

In the limit $t \rightarrow \infty$, we have the following asymptotic result.

$$\lim_{t \rightarrow \infty} M(t)/t \rightarrow 1/\mu \quad (56)$$

where

$$\mu = E[X] = \int_0^{\infty} x dG(x) \quad (57)$$

6.3 Case Study I [Cont.] (Component Reliability)

In Section 6.7 of Chapter 7 we discussed modelling failure and replacement of an unreliable control element and formulated two models (Models I.1 and I.2).

Model I.1 involved a renewal process formulation and Model I.2 involved an alternating renewal process formulation. In this section we carry out an analysis of Model I.1.

MODEL I.1

We shall assume that the failure distribution $G(x)$ is given by

$$G(x) = \theta(1 - e^{-\rho_1 x}) + (1 - \theta)(1 - e^{-\rho_2 x}) \quad (58)$$

i.e. it is a mixture of two exponential distributions. The density function $g(x)$ ($= dG(x)/dx$) is given by

$$g(x) = \theta\rho_1 e^{-\rho_1 x} + (1 - \theta)\rho_2 e^{-\rho_2 x} \quad (59)$$

To obtain the expected number of replacements over the interval $[0, t]$ we need to evaluate $M(t)$ given by (55). Denoting the Laplace transform of $M(t)$, $G(t)$ and $g(t)$ by $\hat{M}(s)$, $\hat{G}(s)$ and $\hat{g}(s)$ respectively, we have from (55)

$$\hat{M}(s) = \hat{G}(s) + \hat{M}(s)\hat{g}(s) \quad (60)$$

From (58) and (59) we have

$$\hat{g}(s) = \left\{ \frac{\theta\rho_1}{\rho_1 + s} + \frac{(1 - \theta)\rho_2}{\rho_2 + s} \right\} \quad (61)$$

and

$$\hat{G}(s) = \hat{g}(s)/s \quad (62)$$

Substituting (61) and (62) in (60) and simplifying yields

$$\hat{M}(s) = \frac{1}{s^2\mu} + \frac{1}{s} \frac{\sigma^2 - \mu^2}{2\mu^2} - \frac{\theta(1 - \theta)(\rho_1 - \rho_2)^2}{s_1^2(s - s_1)} \quad (63)$$

where

$$s_1 = -\{(1 - \theta)\rho_1 + \theta\rho_2\} \quad (64)$$

and μ and σ^2 are the mean and variance of X . On taking the inverse Laplace transform, we have

$$M(t) = \frac{t}{\mu} + \frac{\sigma^2 - \mu^2}{2\mu^2} - \frac{\theta(1 - \theta)(\rho_1 - \rho_2)^2}{s_1^2} e^{-s_1 t} \quad (65)$$

Note, that as $t \rightarrow \infty$ we obtain the relationship given by (56).

7 Continuous State/Discrete Time Formulations

In Section 7 of Chapter 7 we discussed a fairly general continuous state/discrete time formulation. However, in this section we confine our attention to the analysis of a special formulation discussed in Section 7.3 of Chapter 7.

The variable X_t of the formulation is given by the relation

$$X_t = Y_t + V_t \quad (66)$$

with Y_t a known deterministic sequence and V_t an unknown stochastic sequence generated by a linear difference equation of the form

$$V_t = \sum_{j=1}^n \alpha_j V_{t-j} + \sum_{j=0}^m \beta_j W_{t-j} \quad (67)$$

with W_t being a sequence of independent and identically distributed Gaussian random variables with zero mean and variance σ^2 .

Since the Gaussian property is preserved under linear operation, V_t is a correlated Gaussian sequence, the probabilistic characterization of V_t can be given through its first two moments. We shall confine our attention to V_t being a stationary process with the first moment (viz. $E[V_t] = 0$) and the second moment (viz. $E[V_t V_{t+j}]$) given by

$$v(j) = E[V_t V_{t+j}]. \quad (68)$$

As a result, X_t is also a correlated Gaussian sequence, with

$$E[X_t] = Y_t \quad (69)$$

and

$$E[(X_t - Y_t)(X_{t+j} - Y_{t+j})] = v(j)$$

Expressions for $v(j)$ can be obtained in terms of the parameters of the difference equations given by (67). The $v(j)$ values satisfy a set of linear algebraic equations known as Yule-Walker equations. If $n = 0$ (i.e. V_t is a MA process) then $v(j)$ is identically zero for $|j| \geq m$. If $n \neq 0$ (i.e. V_t is either an autoregressive process if $m = 0$ or an autoregressive moving average process if $m \neq 0$) $v(j)$ is non-zero for all j and when j becomes large it is a decreasing sequence in j .

The behaviour of $v(j)$ as a function of j plays an important role in the selection of n and m of (67) in time series modelling. We shall discuss this aspect in Chapter 16 where we study in detail a case study involving time series modelling.

8 Continuous State/Continuous Time Formulations

The continuous state/continuous time formulations were briefly discussed in Section 8 of Chapter 7. In this section we confine our attention to analysis of two specific types of formulations, both of which have Markov property. The first formulation involves a Weiner process and the results of the analysis will be used in the next chapter in the context of Monte Carlo method for solving parabolic partial differential equations. The second formulation is of relevance in the context of Case Studies I and J.

8.1 Differential Equation Formulations with Wiener Process

A general formulation is given by $X(t)$ satisfying the following differential equation

$$dX(t) = f_1(X(t), t)dt + f_2(X(t), t)dW \quad (70)$$

where $W(t)$ is the standard Wiener process. The initial condition $X(0)$ is uncertain and characterized through a density function $p(x, t_0)$, i.e.

$$\text{prob}\{x < X(0) \leq x + \delta x\} = p(x, t_0)\delta x + o(\delta x) \quad (71)$$

and we assume that $X(t)$ is unconstrained.

Let $p(x, t)$ be the density function characterizing $X(t)$, i.e.

$$\text{prob}\{x < X(t) \leq x + \delta x\} = p(x, t)\delta x + o(\delta x) \quad (72)$$

Then it can be shown (we omit the details) that $p(x, t)$ satisfies the following partial differential equation:

$$\frac{\partial p(x, t)}{\partial t} = \frac{1}{2} \left\{ \frac{\partial^2}{\partial x^2} [f_2^2(x, t) p(x, t)] - \frac{\partial}{\partial x} [f_1(x, t) p(x, t)] \right\} \quad (73)$$

with

$$\text{I.C.: } p(x, t_0) \text{ as specified,}$$

and

$$\text{B.C.: } p(x, t) \rightarrow 0 \text{ as } |x| \rightarrow \infty \quad (74)$$

Note that the B.C. will change if the process is constrained; e.g. $X(t)$ must always lie in the interval $[a, b]$.

In general, it is not possible to solve (73) analytically. For the special case

$$f_2(x, t) = \sigma^2; \quad f_1(x, t) = -\beta x \quad \text{and} \quad p(x, t_0) = \delta(x) \quad (75)$$

an analytic solution exists and is given by

$$p(x, t) = \frac{1}{\sqrt{2\pi D(t)}} e^{-x^2/2D(t)} \quad (76)$$

where

$$D(t) = \sigma^2(1 - e^{-2\beta t})/2\beta \quad (77)$$

As $t \rightarrow \infty$, $D(t) \rightarrow \sigma^2/2\beta$ and $p(x, t) \rightarrow p^*(x)$, the steady state probability density function for $X(t)$.

Note that we could have obtained (76) more directly by noting that under (75) the differential equation is linear, as a consequence of which $X(t)$ is Gaussian. Thus $X(t)$ is completely characterized through its first two moments. The first moment is zero and the second moment $M_2(t)$ is given by the equation

$$dM_2(t)/dt = -2\beta M_2(t) + \sigma^2$$

with

$$M_2(0) = 0 \quad (78)$$

This yields $M_2(t) = D(t)$ given by (77).

8.2 Compound Poisson Process Formulations

The compound Poisson process formulation was discussed briefly in Section 8.3 of Chapter 7. The variable $X(t)$ is given by

$$X(t) = \sum_{i=1}^{N(t)} Z_i \quad (79)$$

where Z_i is a sequence of independent and identically distributed random variables with a density function of $g(z)$, and $N(t)$ is a stationary Poisson process with parameter λ and independent of Z_i .

Let $p(x, t)$ denote the density function of $X(t)$, and let $p(x, t|n)$ be the density function of $X(t)$ conditioned on $N(t) = n$.

Conditioned on $N(t) = n$, $X(t)$ is a sum of n independent random variables, as a result of which we have $p(x, t|n)$ given by a n -fold convolution, i.e.

$$p(x, t|n) = g(x)^* g(x)^* \dots * g(x) \quad (80)$$

where $*$ is the convolution operator. On removing the conditioning, we have

$$p(x, t) = \sum_{n=0}^{\infty} p(x, t|n) \text{prob}\{N(t) = n\} \quad (81)$$

$$= \sum_{n=0}^{\infty} p(x, t|n) \frac{(\lambda t)^n e^{-\lambda t}}{n!} \quad (82)$$

Using characteristic function $\Phi(\theta, t)$ defined as

$$\Phi(\theta, t) = E\{e^{i\theta X(t)}\}$$

we have it equal

$$= \sum_{n=0}^{\infty} \Psi\{(\theta)\}^n \left\{ \frac{(\lambda t)^n e^{-\lambda t}}{n!} \right\} \quad (83)$$

where

$$\Psi(\theta) = E\{e^{i\theta z}\} = \int_{-\infty}^{\infty} e^{i\theta z} g(z) dz \quad (84)$$

and from this we have the following result,

$$\frac{\partial p(x, t)}{\partial t} = -\lambda p(x, t) + \lambda \int_{-\infty}^{\infty} p(y, t) g(x - y) dy \quad (85)$$

Thus the probabilistic characterization of $X(t)$, i.e. $p(x, t)$, can be obtained by solving (85).

THE FIRST PASSAGE TIME

Let τ represent the time for $X(t)$ to reach or cross a barrier at $x = L$. We shall confine our attention to the case where the Y_i values are non-negative. In this it is impossible for the process $X(t)$ to recross the barrier and hence

$$\tau > t \quad \text{if and only if } X(t) < L \quad (86)$$

Let $q(v, L)$ denote the density function of τ . Then from (86) we have

$$\int_t^\infty q(v, L) dx = \int_0^L p(x, t) dx \quad (87)$$

or

$$1 - \int_0^t q(v, L) dx = \int_0^L p(x, t) dx \quad (88)$$

Using transform techniques it is possible to obtain expressions for $q(v, L)$; we illustrate this in a later subsection.

8.3 Case Study J [Cont.] (Speed of Aeroplanes)

In Section 8.5 of Chapter 7 we formulated two models (Models J.4 and J.5) for predicting $X(t)$, the maximum speed of aeroplanes. Both these models use compound Poisson process formulations as dummies. In this section we carry out an analysis of Model J.4.

MODEL J.4

We assume that the density function characterizing the changes to the maximum speed with each breakthrough is exponential, i.e.

$$g(z) = \rho e^{-\rho z} \quad (89)$$

As a result the density function for $X(t)$ conditioned on $N(t) = n$ is given by (80). On taking the Laplace transform with respect to x we have

$$\begin{aligned} \hat{p}(s, t|n) &= \mathbb{E}\{p(x, t|n)\} \\ &= [\hat{g}(s)]^n = \{\rho/(\rho + s)\}^n \end{aligned}$$

Using this in (82) gives

$$\hat{p}(s, t) = \mathbb{E}\{p(x, t)\} = \sum_{n=0}^{\infty} \left(\frac{\rho}{\rho + s} \right)^n \frac{(\lambda t)^n e^{-\lambda t}}{n!} = e^{-\lambda t} \exp\left(\frac{\rho \lambda t}{\lambda + s}\right) \quad (90)$$

On taking the inverse Laplace transform, we have

$$p(x, t) = e^{-\lambda t} \delta(x) + \sqrt{(\rho \lambda t/x)} e^{-(\lambda t + \rho x)} I_1(2\sqrt{\rho x \lambda t}) \quad (91)$$

where $\delta(x)$ is the delta function and $I_1(\cdot)$ is a Bessell function of imaginary argument.

From this, expressions for the various moments of $X(t)$ can be obtained. In particular, the mean $M(t)$ and the variance $\sigma^2(t)$ are as follows:

$$M(t) = \lambda t / \rho \quad (92)$$

and

$$\sigma^2(t) = \lambda t(1 + \rho) / \rho$$

From (92) we see that both the mean and the variance of $X(t)$ increases linearly with t . Note that we could have derived the expression for $M(t)$ more easily by noting that on the average one breakthrough occurs every $1/\lambda$ units of time, and the average increase per breakthrough ($= E(Z)$) is $1/\rho$. As a result, at time t the mean value of $X(t)$ is given by the expression in (92).

8.4 Case Study I [Cont.] (Component Reliability)

In Section 8.4 of Chapter 7 we formulated a model (Model I.3) for characterizing the time to failure. The variable of the model, $X(t)$, represents the crack length. $X(t)$ changes as described in Section 8.3 and failure occurs when it crosses a level L . In other words, the time to failure is given by τ , and we seek the density function $q(v, L)$ for it.

We shall assume that the increase in crack length with each shock is given by an exponential density function, i.e. $g(z)$ is given by (89).

The density function $q(v, L)$ can be obtained from (88). On taking the Laplace transform with respect to t , we have

$$\{1 - \hat{q}(a, L)\} / a = \int_0^L \hat{p}(x, a) dx \quad (93)$$

where

$$\begin{aligned} \hat{q}(a, L) &= \int_0^\infty q(t, L) e^{-at} dt \\ \hat{p}(x, a) &= \int_0^\infty p(x, t) e^{-at} dt \end{aligned} \quad (94)$$

Rearranging (93) yields

$$\hat{q}(a, L) = 1 - a \int_0^L \hat{p}(x, a) dx \quad (95)$$

Taking Laplace transform with respect to L we have

$$\tilde{q}(a, s) = \{1 - \tilde{p}(s, a)\} / s \quad (96)$$

where

$$\begin{aligned} \tilde{q}(a, s) &= \int_0^\infty \hat{q}(a, L) e^{-sL} dL \\ \tilde{p}(s, a) &= \int_0^\infty \hat{p}(x, a) e^{-sx} dx \end{aligned} \quad (97)$$

$\tilde{p}(s, a)$ can be obtained from (90) by taking the Laplace transform with respect to t . On substituting this into (96) we have

$$\tilde{q}(a, s) = \lambda / \{\rho\lambda + a\mu + as\} \quad (98)$$

On taking the inverse transforms, we have

$$q(v; L) = e^{-\lambda v - \mu L} \sum_{m=0}^{\infty} \frac{\lambda^{m+1} v^m (\mu L)^m}{m! m!} = \lambda e^{-\lambda v - \mu L} I_0\{2\sqrt{\lambda v \mu L}\} \quad (99)$$

where $I_0(\cdot)$ is a Bessel function of imaginary argument. This gives the probability density function for the time to failure.

From (99) we can obtain the various moments of τ . In particular, the first moment (or the mean time to failure) is given by

$$E[\tau] = \int_0^{\infty} v q(v, L) dv = (1 + L)/\mu. \quad (100)$$

Similarly, other moments can be obtained.

Notes and References

Our presentation has been very terse. For further details of analysis of different types of stochastic processes see the books mentioned in Chapter 7.

The derivation of the results of Section 4 can be found in most books on stochastic processes (e.g. [1]) or any book on Markov chains. More advanced books on Markov chains deal with specialized topics – e.g. [2] deals with the analysis when the states are aggregated, [3] with the analysis of various level-crossing problems.

Item [4] contains details of derivation for a variety of queueing processes. For further details of the derivation of the results of Section 6 see [5] and [6].

Details of analysis of stochastic differential equations (Section 8.1) can be found in [7], which also examines the case where $X(t)$ is constrained to lie in a specified interval. For level-crossing problems associated with continuous state/continuous time processes, see [8]. Item [5] gives details of the derivations of Sections 8.2–8.4 for the compound Poisson process.

Stationary stochastic processes can be analysed either in time domain or in frequency domain. The latter method of analysis is called the “spectral method of analysis”; further details of it can be found in [9] and [10].

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CHAPTER 9

Simulation

1 Introduction

In Chapter 5 we discussed a variety of deterministic formulations, and in Chapter 7 a variety of stochastic formulations suited to modelling systems. To obtain model behaviour we examined the analysis of these two classes of formulations in Chapters 6 and 8 respectively. Unfortunately only a small class of formulations can be solved by analytical methods. For the majority of formulations the solution can be obtained only by means of some computational method. In Chapter 4 (Section 5.2) we mentioned that the implementation of a mathematical model on a computer to obtain the behaviour is called "simulation", and the computer with the instructions to implement the model a "simulator".

In Chapter 6 we indicated the different types of computers useful in solving mathematical formulations. We went on to discuss some specific techniques for solving deterministic formulations on digital computers without going into the implementation details. In a sense those solution procedures can be regarded as a part of digital computer simulation of systems describable by deterministic formulations.

In this chapter we focus our attention on the implementation of a model on a computer to obtain the model behaviour. Both analog computer simulations and digital computer simulations will be discussed.

The simulation procedure depends on the nature of the underlying mathematical formulation. Simulation techniques can be divided into different categories depending on whether changes in the model occur continuously over time or only at discrete points in time, and whether the changes are deterministic or stochastic. The translation of a model (or more correctly the underlying mathematical formulation) into a program for implementation on a digital computer can be done using a variety of languages. We shall review some of the more widely used languages and briefly discuss two of them. Finally, we conclude with a brief discussion of Monte Carlo methods. These methods yield approximate estimates of the solution for a variety of deterministic formulations by computer experimentation.

2 Analog Computer Simulation

The analog computer is ideally suited to simulating deterministic models involving ordinary differential equation formulations. They can be used, less effectively, for simulating models involving other types of deterministic formulations and stochastic formulations. However, we shall confine our attention to simulating models involving ordinary differential equation formulations.

2.1 Principles of Analog Simulation

As mentioned in Chapter 6 (Section 3.2), an analog computer consists of a variety of components (or blocks) – each characterized by one or more input voltages and an output voltage. The output and input voltages can change with time and are related by some mathematical relationships (e.g. addition, multiplication, division, integration). By linking different components (also called *patching*) the voltages become related and satisfy some algebraic and/or differential equation.

If the underlying formulation of a model is an ordinary differential equation then, by suitable patching, the differential equation satisfied by the voltages in the analog computer simulation can be made identical to a scaled version of the given differential equation. Thus the time history of one or more voltages corresponds to the solution of the differential equation and hence constitutes the behaviour of the model.

2.2 Procedure for Simulation

The procedure for simulating a model describable in terms of an ordinary differential equation formulation is given by the following four steps.

Step 1: Scaling the equation. This involves rewriting the given differential equation in terms of non-dimensional variables, as discussed in Section 4.3 of Chapter 6. Note that this involves scaling both the independent variable and all the dependent variables and their derivatives.

Step 2: Drawing the patching diagram. This is a flow diagram which shows the connection between different components of the analog computer so that the equation relating the voltage is identical to the scaled equation of step 1. The diagram is drawn using special symbols for the different components; a short list of symbols is given in Figure 9.1.

Step 3: Patching and checking. Patching involves connecting different components using wires (also called patching cords) according to the patching diagram. Checking is a procedure to test if the patching is in agreement with the patching diagram.

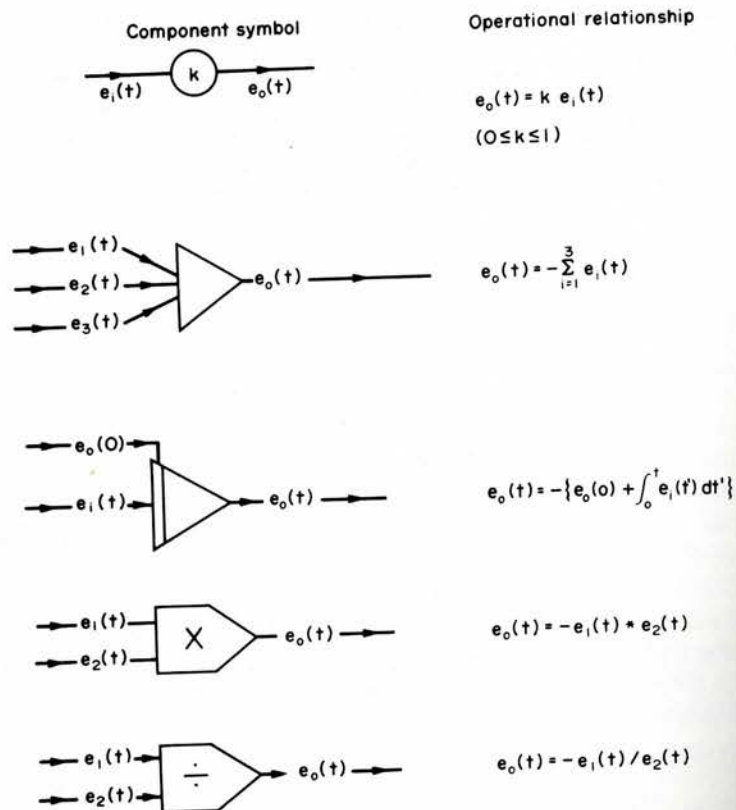


FIGURE 9.1 A sample of component symbols used in patching for analog simulation.

Step 4: Running the computer. This corresponds to initiating the sequence of operations to generate the solution and hence the behaviour of the model.

2.3 Case Study E [Cont.] (World Population)

In Section 5.5 of Chapter 5 we proposed three models (Models E.4 to E.6) involving ordinary differential equation formulations. In this section we examine simulating Model E.5 (i).

MODEL E.5 (i)

The model is given by

$$N'(t) = dN(t)/dt = \theta\{L - N(t)\}N(t) \quad (1)$$

where $N(t)$ represents the total population at time t and the initial condition

given by

$$N(t_0) = N_0 \quad (2)$$

Step 1: Scaling. Let N_m and N'_m represent the maximum values of $N(t)$ and $N'(t)$ respectively. Define $n(t)$ and $n'(t)$ as follows:

$$n(t) = N(t)/N_m \quad \text{and} \quad n'(t) = N'(t)/N'_m \quad (3)$$

These are the scaled variables and using (3) in (1) we have

$$n'(t) = \{N_m/N'_m\}\theta N_m\{L/N_m - n(t)\}n(t) \quad (4)$$

Note that

$$\int n'(t) dt \neq n(t) \quad (5)$$

but

$$= \{N_m/N'_m\}n(t) \quad (6)$$

Since L is the upper limit for $N(t)$, we select $N_m = L$. We also consider a transformation of the independent variable t to τ such that

$$t = \beta\tau \quad (7)$$

This results in (4) getting transformed into

$$dn(\tau)/d\tau = \delta\{1 - n(\tau)\}n(\tau) \quad (8)$$

where

$$\delta = \beta\theta L \quad (9)$$

We select β to ensure $\delta < 1$. Finally, the initial condition is given by

$$n(t_0) = n_0 = N_0/L \quad (10)$$

Step 2: Patching diagram. The patching diagram is as shown in Figure 9.2.

We omit the details of steps 3 and 4. The simulation results for $n(\tau)$ are as shown in Figure 9.3 for two values of δ . From this we can obtain $N(t)$ using (3) and (7) for two values of θ , as θ and δ are related by (9).

3 Digital Computer Simulation

We shall first consider simulating models involving deterministic formulations, and later the simulation of models involving stochastic formulations.

3.1 Deterministic Model Simulation

If the model to be simulated involves difference equation formulations (i.e. changes to the variables of the model occur at discrete points in time) then simulating the model on a digital computer is fairly easy. The difference

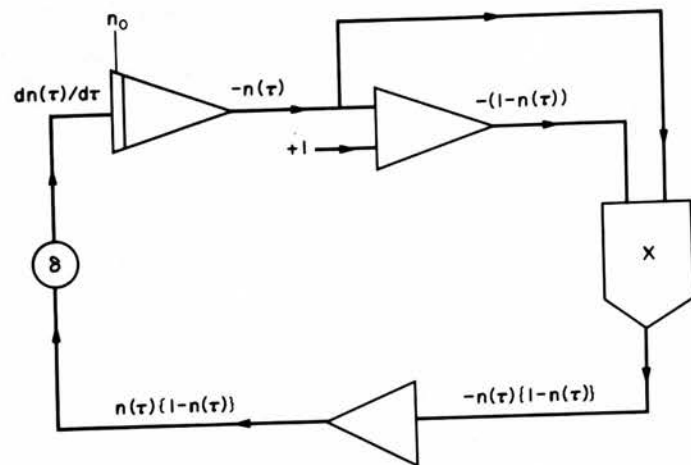
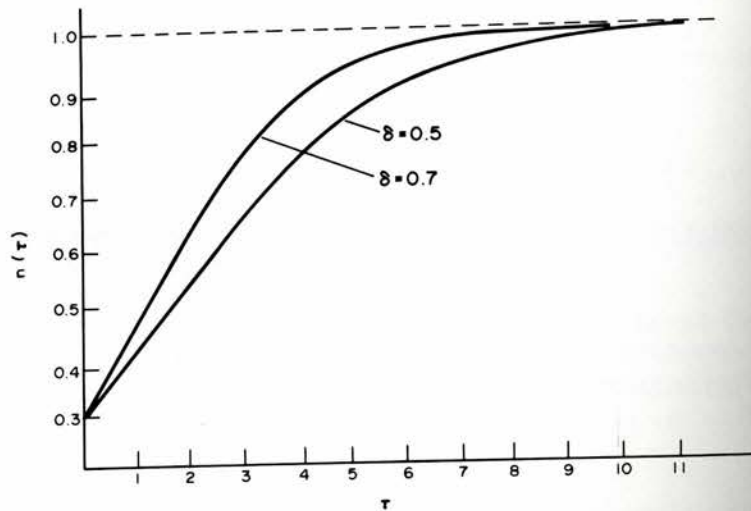


FIGURE 9.2 Patching diagram for Model E.5.

FIGURE 9.3 Plot of $n(\tau)$ for two values of δ for Model E.5.

equation can be viewed as a recursive relationship, and the solution (and hence the model behaviour) obtained by a simple recursive scheme which can be easily implemented. When the model involves either ordinary differential equation or partial differential equation formulations, then the behaviour cannot be obtained as a continuous function of time (time or spatial variables in the case of partial differential equation) because of the nature of the digital computer. However, as discussed in Section 3.1 of Chapter 6, the solution can

be obtained for discrete values of variables by treating the continuous flow of the variable by an approximation where the variable is incremented in small steps. The study of algorithms to obtain the solution for discrete values of time (time and spatial variables) in the case of ordinary (partial differential) equations belongs to the theory of numerical analysis. We shall not discuss this aspect here, but instead confine our attention to computer implementation.

The computer implementation of a model can be done using either a general-purpose language (e.g. Fortran, Pascal) or a special simulation language (e.g. CSMP, Dynamo) designed for specific model types. The implementation using a general-purpose language requires the user to supply the following programs:

- (i) program to define model formulation,
- (ii) program to generate solution,
- (iii) program to display solution and
- (iv) main program to execute (i)–(iii).

As a result it requires a lot of programming from the user. The programming effort can be substantially reduced if a specially designed language is used, in which case the user has to write a program to define the model formulation and the special language takes care of the rest.

3.2 Stochastic Model Simulation

We shall confine our discussion to simulating stochastic models where changes occur at discrete points in time – as in the case of discrete time models (with continuous or discrete states) or continuous time models with discrete states. The simulation of stochastic models differs from deterministic models in one important sense. In stochastic model simulation each simulation yields a different time history of model behaviour. This is to be expected, as each time history corresponds to a particular outcome (or realization) of the underlying stochastic process formulation.

The simulation of a stochastic model requires generation of random numbers, updating the clock (which represents the time variable of the model) and other variables using the random numbers generated earlier; plotting or displaying the time history of model behaviour and finally compiling the statistics of the model behaviour based on a specified number of independent simulations. Since it is not possible to generate truly random numbers, simulation of stochastic models is done by using pseudo-random numbers generated by algorithms. A variety of such random-number generators have been developed for generating random numbers with specific statistical properties.

As in the case of deterministic model simulation, the computer

implementation of a stochastic model can be done using either a general-purpose language or a special simulation language (e.g. GPSS, SIMSCRIPT) designed for specific model types. We shall review some of these special languages in a later section. We illustrate the principles of stochastic model simulation by considering the following case study.

3.3 Case Study K [Cont.] (Supermarket Operation)

In Section 6.5 of Chapter 7 we proposed two models (Models K.1 and K.2) for the checkout counter operation. The behaviour of Model K.1 was obtained by analytical methods in Section 5.2 of Chapter 8. It is extremely difficult to obtain the behaviour of Model K.2 by analytical methods. In this section we discuss the use of simulation to obtain the model behaviour.

MODEL K.2

We assume that there are S counters. Customers arrive according to a point process with inter-arrival times being a sequence of independent random variables with a distribution function F . The service times are also independent random variables with a distribution function G . When a customer arrives, the service starts immediately if one of the counters is free. If all the counters are busy the customer joins the queue at the counter which has the least number of people waiting to be served. (If there be more than one such counter, the customer chooses among them randomly. The same is true in the selection of a counter if more than one counter is free at the time the customer arrives.)

The passage of customer through the checkout counter can be described by a flow diagram shown in Figure 9.4, and is the starting point of simulation.

Note that random-number generators are needed to execute blocks 1 and 6 of the flow diagram. In addition, one needs a clock to characterize passage of time and tables to keep track of queue lengths (block 8) and idle times of server (block 10) for each of the S different checkout counters.

A typical plot of the time history is shown in Figure 9.5 for the case of a single counter operation.

4 Digital Simulation Methodology

Since, in digital simulation, the underlying formulation is being implemented as a program on a computer, the nature of a mathematical model suitable for simulation is in general different from that for analytical treatment. When building a model for analysis by analytical methods it is necessary to bear in mind the constraints and limitations of such methods. When a mathematical model is being built for simulation, no such constraint needs to be imposed. Models are built in terms of simple equations and logical expressions, and

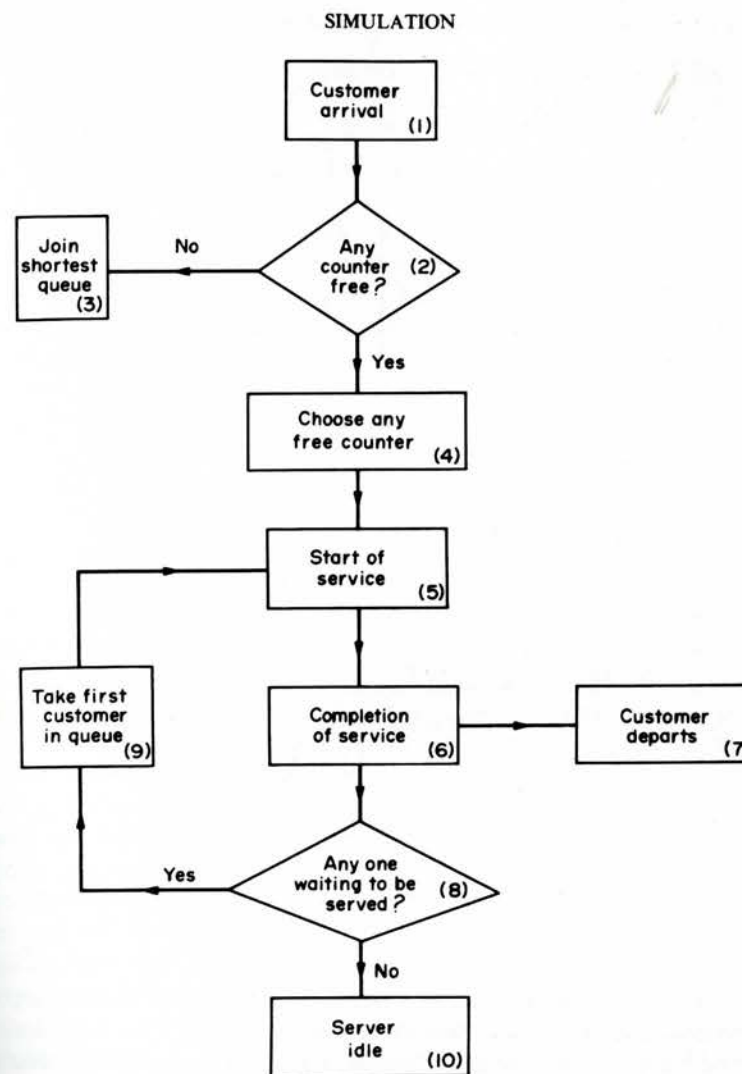


FIGURE 9.4 Flow diagram for simulating Model K.2.

organized in a way that enables a routine procedure to be used to solve them. Typically, they are built by dividing the system into a series of sections. Each section is described in a straightforward manner (using logical expressions and simple mathematical equations) without undue concern for the complexity introduced by having many such sections.

We use the terms "simulation model" and "simulation modelling" to mean the following: a mathematical model developed to study the behaviour of a system by simulation is called a *simulation model* and the process of building such a model is termed *simulation modelling*. As a consequence, a special

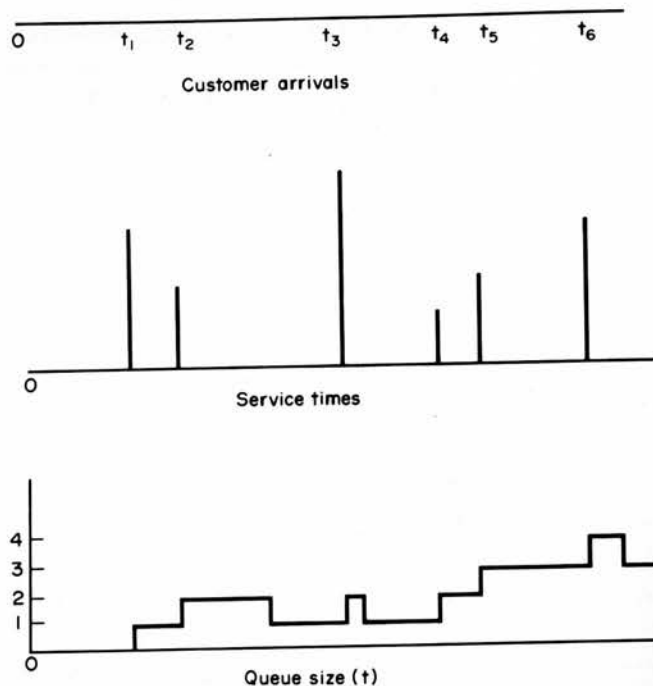


FIGURE 9.5 A simulated model behaviour for Model K.2.

terminology has evolved for use in simulation modelling, which will now be described.

4.1 Brief Introduction to Simulation Terminology

In simulation modelling the system is viewed as consisting of various sections (or subsystems). Each section is described in terms of *entities*, and the term *attribute* denotes a property of the entity. Any process (internal or external) which causes changes in the system over time is called an *activity*. The initiation, alteration or conclusion of an activity is called an *event*. The term *state of the system* is used to mean a description of all the entities, attributes and activities as they exist at one point in time. The evolution of the system is studied by following the changes in the state of the system.

Entities and attributes make up the static structure of a simulation model. They describe the state of a system but not how the system operates. This is the task of activities and events. The key to simulation is the programmer's ability to organize system events so that the order in which they are executed within the computer corresponds to the order in which they would occur in the real system. This preserves the time relationships between simulated and real events.

In the case of Model K.3, discussed in the previous subsection, the servers at the counters would be called entities, customers would be called activities and the arrival and departure of customers would be called events.

The simulation methodology consists of the following two steps:

Step 1: Building the simulation model. This is done by breaking the system into sections and identifying entities, attributes, activities and events.

Step 2: Writing the computer program. This converts the simulation model into a simulation program. It consists of:

- (i) writing a set of event programs to describe the system operating rules;
- (ii) defining lists and matrices that store information; and
- (iii) writing an executive routine that directs the flow of information and control.

4.2 Classification of Simulation

Simulation can be classified into two types: discrete simulation and continuous simulation. In discrete simulation, changes in state occur at discrete points in time. Thus, activities are not modelled explicitly; they are represented by modelling the events that affect the state of the system. In continuous simulation, changes in state occur continuously over time; hence activities need to be modelled explicitly. In both cases the flow of time is recorded by a clock in the simulator.

Since changes over time cannot be represented continuously on a digital computer, time is advanced in small increments to approximate the continuous flow of time in the system being simulated. Thus, in the simulation of continuous systems (i.e. systems modelled by differential equations), the simulation transforms the differential equation formulation into a difference equation formulation.

In discrete simulation, time is broken into intervals. The beginning and end of each interval corresponds to the occurrence of an event. These intervals are not necessarily equal and in the simulation of a stochastic system they are random variables. The flow of time is achieved by updating the clock at time instants at which events occur.

4.3 Event vs Activity Oriented Simulation

In discrete simulation, events and activities play a major role. The key element is the simulation algorithm, which has a structure as shown in Figure 9.6. Basically it involves finding the next potential event – executing if possible. The execution involves advancing the clock (which represents flow of time in the simulation) and changing the state of the system.

In the computer the state is represented by numerical values and is called the

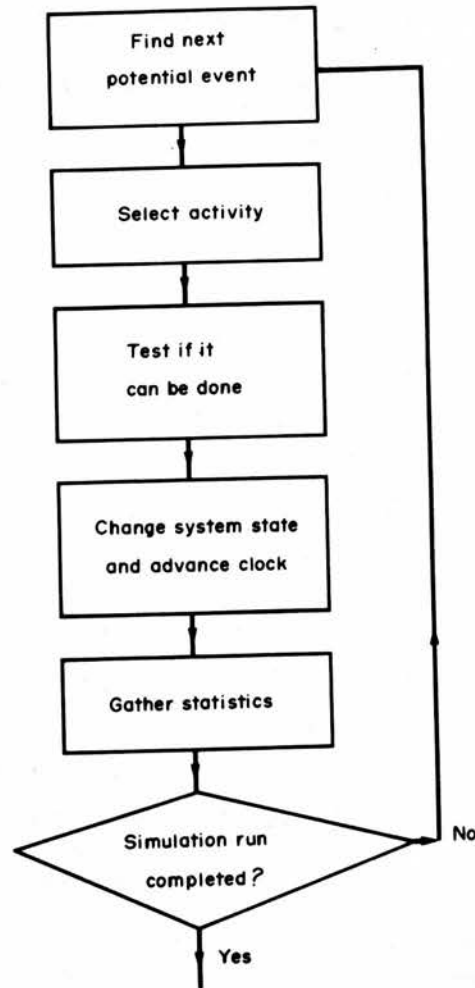


FIGURE 9.6 Simulation algorithm for discrete simulation.

“system image”. Changes in system image over time correspond to behaviour of the simulation model.

The key factor in simulation is the control of sequences that represent changes in the simulation. There are two different ways of executing this control, which lead to two different types of simulation – event-oriented simulation and activity-oriented simulation. In event-oriented simulation the emphasis is on event finding, and the simulation algorithm automatically obtains the next event when all the state changes are completed. In activity-oriented simulation the emphasis is on activity starting and stopping, and this

approach is useful where an activity can start or finish only when many conditions are met.

The subtle difference is that, in event-oriented simulation, the times at which system changes occur are treated as characteristics of the activities, while in activity-oriented simulation these times are treated as attributes of the entities. This difference is important, as some languages are based on the event-oriented approach while others are based on the activity-oriented approach. The difference is in the control of program execution, but the final simulation remains the same.

4.4 Verification and Validation

A simulation model becomes an adequate model once it is validated (i.e. passes the test of validation). In simulation literature, a term called “verification” is often used. Verification is a testing procedure (similar to validation) which establishes the faithfulness of the computer output to the model response. Thus the computer output is in agreement with the system behaviour only when the simulation is verified and validated – i.e. verification establishes that the computer output is in agreement with the simulation model behaviour, and validation establishes that the simulation model is an adequate representation of the system.

5 Simulation Languages

Though almost any type of programming language can be used to implement a simulation model, various special languages have been developed for simulation applications. These languages provide the user with a variety of services; they are designed to ease the job of translating a simulation model into a program to simulate the system behaviour on a computer. They contain: (a) status descriptions, which are definition of the essential element of the model; (b) procedures for modifying the state of a model; and (c) procedures for controlling and observing the model behaviour. In addition to these, extensive error checking exists to prevent misuse of the language, as well as routines for debugging and locating logical errors.

Simulation languages can be divided into three groups as indicated below:

- (i) continuous simulation languages,
- (ii) discrete simulation languages, and
- (iii) combined simulation languages.

It is not possible to discuss all the simulation languages. In the next two subsections we briefly review some of the more widely used languages and comment on their salient features.

5.1 Continuous Simulation Languages

Continuous simulation languages deal with the simulation of continuous time systems, modelled by differential equations, on digital computers in essentially the same way they are solved on analog computers. In a sense, a program to allow this kind of operation converts the digital computer to a digital-analog simulator. This requires an approach similar to that used on an analog computer; e.g. the user constructs functional diagrams which are similar to the patching diagrams used in analog computing.

A number of continuous simulation languages have been developed which offer the user great freedom in modelling a system and translating it into a program. They make use of statements which allow direct programming of the equations of a simulation model and include a variety of algebraic and logical expressions to describe relations between variables. We review two of the many continuous simulation languages to give some idea of the approach taken with this class of simulation language.

5.2 CSMP (Continuous System Modelling Program)

This is specially designed to simulate models involving ordinary differential equations. There is flexibility with regard to the choice of the numerical integration method to be used in the simulation. The language is Fortran-based and is constructed of three types of statements.

- (i) *structural statements* which define the simulation model;
- (ii) *data statements* which assign numerical values to parameters; and
- (iii) *control statements* which specify options for the execution of the program and the choice of output.

The output can be displayed in tabular form and/or printed as plotted graphs.

5.3 Case Study D [Cont.] (Rocket Launch)

The model formulation for this problem was done in Section 5.4 of Chapter 5, where we discussed the solution by analytical methods. The model is given by

$$x''(t) = -(k/M)x'(t) - \{g_0 R^2\}/(x(t) + R)^2 \quad (11)$$

with the initial conditions given by

$$x(0) = 0 \quad \text{and} \quad x'(0) = v \quad (12)$$

For simulating the model using CSMP we need to rewrite (11) as a system of first-order ordinary differential equations. This is done by the technique discussed in Section 5.2 of Chapter 5.

Define

$$y(t) = x'(t) \quad (13)$$

Then (11) can be rewritten as

$$\begin{aligned} x'(t) &= y(t) \\ y'(t) &= -(k/M)y(t) - \{g_0 R^2\}/(x(t) + R)^2 \end{aligned} \quad (14)$$

with initial conditions given by

$$x(0) = 0 \quad \text{and} \quad y(0) = v \quad (15)$$

The computer program for simulating the model in CSMP is shown in Figure 9.7.

We briefly comment on the various statements of the program.

- (i) The first statement defines the title.
- (ii) The next two statements define the equations of the model.
- (iii) INTGRL (X0, XDOT) is a statement to integrate x starting with an initial value $X0$.
- (iv) CONST defines the numerical values for the parameters and the initial conditions.
- (v) TIMER defines the parameters for integration. The terms used stand for
DELTA: Integration interval
FINTIM: Finish time
PRDEL: Interval at which to print results
- (vi) PRINT defines that both $X(t)$ and $Y(t)$ are to be printed.
- (vii) PARAM is a statement to repeat the simulation with different values of $Y0$ as indicated.

5.4 DYNAMO

In simulating with this language the model is broken down into a number of reservoirs, or "levels", interconnected by flow paths. A level represents the

```
TITLE  ROCKET LAUNCH
XDOT = Y
YDOT = -(K/M)*Y - G0*R**2/(X+R)**2
X = INTGRL (X0, XDOT)
Y = INTGRL (Y0, YDOT)
CONST  K =      , M =      , G0 =
        R =      , X0 =      , Y0 =
TIMER  DELT = 0.1, FINTIM = 500, PRDEL = 10.0
PRINT  X, Y
PARAM  Y0 = ( . . . . )
END
```

FIGURE 9.7 Program of simulating Model S.1 using CSMP.

accumulation of an entity, and corresponds to the accumulated difference between the input and output flows for that entity. The instantaneous flows are represented by "rates". The rate is related to the level by the expression

$$\text{Rate} = \text{level}/\text{delay}$$

where the "delay" is a characteristic time. Thus, if $x(t)$ represents the level of an entity and its rate be given by

$$dx(t)/dt = -x(t)/T \quad (16)$$

then T represents the "delay". The smaller the value of T (or delay), the greater is the rate, and vice-versa.

As in CSMP, output can be in the form of tables and/or printed plotted graphs.

5.5 Discrete Simulation Languages

In Section 4.3 we discussed two ways (event-oriented and activity-oriented) of implementing discrete simulation. Two other ways of implementation are process-oriented and transaction flow. Unfortunately, the terminology is not consistent. As mentioned earlier, there are a large number of simulation languages; each uses one of the above-mentioned four ways for implementation of the simulation. The most commonly used languages are GPSS, SIMSCRIPT, GASP and SIMULA.

5.6 GPSS (General-Purpose System Simulator)

This is a process-oriented-type discrete event simulation language. It is a block diagram language. A number of basic block types are defined, each representing a particular action. The user must describe the activities of the system in terms of these basic block types. Permanent entities are identified with predefined concepts such as facilities, storages and logic switches. The sequence of activities is established by a block diagram indicating how the blocks are interconnected and, where necessary, the conditions for a choice between alternative paths. With this the GPSS is able to establish a system image as a set of well-defined tables. Finally, the gathering of statistics is controlled by certain block types together with internal routines. A fixed report generator gives the desired statistics. The language allows for editing the output with explanatory comments.

5.7 Case Study K [Cont.] (Supermarket Operation)

The model building for this problem was done in Section 6.5 of Chapter 7, and in Section 3.3 we briefly discussed the simulation of Model K.2.

In this section we give the program to simulate Model K.2 using GPSS for

$S = 1$, i.e. there is only one checkout counter. The simulation for $S > 1$ is slightly more complicated as it requires more conditional testing. We assume that the interval arrival time for customers is a random number uniformly distributed between 70 and 130, and that the customer service is also a random number uniformly distributed between 50 and 90.

As mentioned earlier, GPSS is a block diagram simulation language. The first step in the simulation is to describe the model in terms of the basic blocks. This is done in Figure 9.8, which shows the flow chart as well as the GPSS block diagram for the model. The GPSS program is given in Figure 9.9.

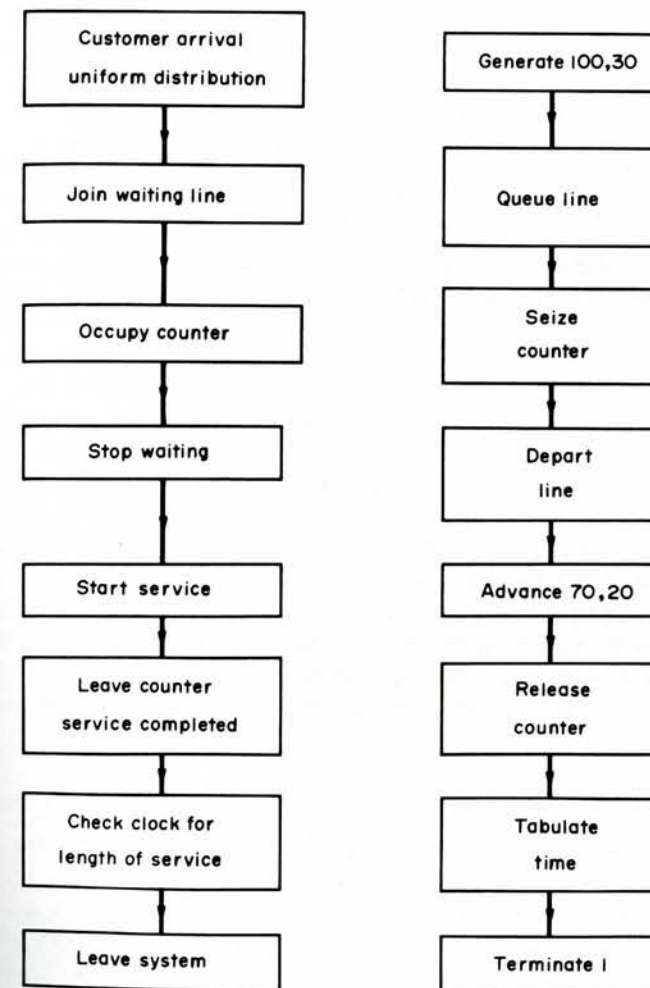


FIGURE 9.8 Flowchart and GPSS block diagram for Model K.2.

	GENERATE	100,30	(1)
	QUEUE	LINE	(2)
	SEIZE	COUNTER	(3)
	DEPART	LINE	(4)
TIME	ADVANCE	70,20	(5)
	RELEASE	COUNTER	(6)
	TABULATE	XTIME	(7)
	TERMINATE	1	(8)

FIGURE 9.9. Program for simulating Model K.2 using GPSS.

We briefly comment on some of the statements of the program.

- (i) The program uses eight different block types (as shown in the right half of Figure 9.8).
- (ii) The queue formed is labelled "LINE" and the service facility "COUNTER".
- (iii) GENERATE creates inter-arrival times.
- (iv) ADVANCE creates service times.
- (v) SEIZE and RELEASE modify the status of service facility.
- (vi) TABULATE is for accumulation and printing of information and the table used is labelled XTIME.

5.8 SIMSCRIPT

SIMSCRIPT is an event-oriented simulation language. In simulating with SIMSCRIPT each type of entity is individually defined by giving names to entities and to their attributes, and specifying their data structure. The activities are represented by individually written routines (called event routines) written in the SIMSCRIPT language. The linking of activities is carried out by event notices, which are also individually defined by the user. Each event notice corresponds to an event due to occur at a particular time. It identifies the activity (event routine) to be activated by an event notice, and the user must create further event notices for scheduling follow-on events. A separate form is used to describe the output required from the program, allowing extensive editing of the results.

5.9 GASP

This is a combined simulation language – i.e. it allows for simulating models where changes occur continuously with time as well as occurring at discrete points in time. Changes occurring discretely are described through entities; associated variables and sets which are referred to as a file. Changes occurring continuously are described through state variables. The dynamic behaviour is described by means of two types of events – time events and state events. The former are scheduled to take place at future points in time, while the latter

occur whenever a state variable meets some prescribed condition. A user-written routine needs to be supplied for each type of event. In addition, GASP offers a range of packages for data gathering and reporting.

5.10 SIMULA

This is a process-oriented type discrete event simulation language. The model to be simulated is viewed as consisting of a collection of processes. The actions and interaction of the processes comprise the dynamic behaviour of the model. The process is an entity which can exist in one of four states – active, suspended, passive and terminated. For each process the user must supply a routine that describes the process. In SIMULA, future processes are sequenced in a sequencing set according to their time attribute. The language also provides packages for the collection of statistics.

6 Monte Carlo Method

In Chapter 6 we discussed analytical and numerical techniques for solving deterministic formulations. An alternative technique, useful in solving certain types of deterministic formulations, is one which can be termed "experimental mathematics". A properly designed experiment using random numbers is carried out many times on a computer. The outcome (a random variable) of each experiment is noted. The solution to the deterministic formulation is given in terms of an estimate based on these outcomes. The estimated solution is a random quantity, characterized by mean and variance. If the experiment is properly designed the estimated solution has mean equal to the true solution and a small variance, thus making it meaningful. In general, the variance goes down as $1/N$ where N is the number of times the experiment is repeated. Hence by choosing a large N the estimated solution is fairly close to the true solution.

The technique is applicable only when a suitable experiment can be devised so that the outcome of the experiment can be related to the true solution. This technique is known as the *Monte Carlo Method*.

We illustrate by giving two examples.

Example 1

The problem is to evaluate the integral

$$I = \int_a^b f(x) dx \quad (17)$$

where $f(x)$ is a specified function. For simple forms of $f(x)$ the integral can be evaluated analytically. For any arbitrary form of $f(x)$ the integral can be evaluated by one of many numerical methods. A Monte Carlo method to obtain an estimate of I is given by the following algorithm.

- (1) Generate a sequence U_i , $1 \leq i \leq N$, from a uniform distribution over $[0, 1]$
- (2) Compute $X_i = a + U_i(b - a)$, $1 \leq i \leq N$.
- (3) Compute $f(X_i)$, $1 \leq i \leq N$.

(4) Compute the estimate $\tilde{I}$ by

$$\tilde{I} = (b-a) \left\{ \sum_{i=1}^N f(X_i) \right\} / N \quad (18)$$

Then it can be shown that

$$E[\tilde{I}] = I \quad (19)$$

and

$$\text{var}[\tilde{I}] = \left[(b-a) \int_a^b f^2(x) dx - I^2 \right] / N \quad (20)$$

indicating that the variance $\rightarrow 0$ as $N \rightarrow \infty$.

The above method is called the "Simple-Mean" Monte Carlo method and is one of many methods for evaluating such integrals.

Example 2

Consider the parabolic equation

$$\partial/\partial t \{U(x, t)\} = (1/2) \partial^2/\partial x^2 \{ \alpha^2(x, t) U(x, t) \} + \partial/\partial x \{ \beta(x, t) U(x, t) \} \quad (21)$$

with the I.C. and B.C. given by

$$\text{I.C.: } U(x, 0) = \delta(x) \quad \text{B.C.: } U(x, t) \rightarrow 0 \text{ as } |x| \rightarrow \infty \quad (22)$$

This equation can be easily solved by numerical methods. We will illustrate the use of the Monte Carlo simulation technique to obtain the solution $U(x, t)$ for some specified $t = t^*$.

Consider a stochastic differential equation given by

$$dZ(t) = \beta(Z, t)dt + \alpha(Z, t)dW(t), \quad Z(0) = 0 \quad (23)$$

where $W(t)$ is the standard Weiner process. From Section 8.1 of Chapter 8 we have that the probability density function $p(z, t)$ of $Z(t)$ satisfies the equation

$$\partial/\partial t \{p(z, t)\} = (1/2) \partial^2/\partial z^2 \{ \alpha^2(z, t) p(z, t) \} + \partial/\partial z \{ \beta(z, t) p(z, t) \} \quad (24)$$

with

$$\begin{aligned} \text{I.C.: } p(z, 0) &= \delta(z) \\ \text{B.C.: } p(z, t) &= 0 \text{ as } z \rightarrow \pm \infty \end{aligned} \quad (25)$$

Thus we see that $p(z, t)$ is identical to $U(x, t)$. Hence once $p(z, t^*)$ is obtained, we have the desired solution $U(x, t^*)$; $p(z, t^*)$ can be obtained using Monte Carlo simulation as follows.

The stochastic differential equation is simulated until time $t = t^*$ starting with an I.C., $Z(0) = 0$. The value of $Z(t^*)$ is noted; let this be denoted by z_1 . The experiment is repeated N times to yield $z_2, z_3, \dots, z_N$ where z_i is the value of $Z(t^*)$ for the i th experiment. From histogram plot of the observed values an estimate of $p(z, t^*)$, and hence of $U(x, t^*)$, can be obtained. The larger the value of N , the smaller the uncertainty – in other words, the more accurate the estimated solution.

Notes and References

Items [1]–[5] show a small sample of the large number of books on simulation modelling and analysis. Most simulation books discuss the different aspects of simulation – viz. modelling, verification, validation etc. Item [6] develops a formal theory for simulation modelling and [7] is an example of the large number of books dealing with statistical aspects of simulation.

Discrete system simulation has received more attention than continuous system simulation. For further details of simulating continuous systems, see [8]; of CSMP, see [9] and of DYNAMO, see [10].

For more on discrete system simulation see [11]. Details of specific simulation languages can be found in many books devoted to the topic; [12]–[17] are a small sample.

Our presentation of Monte Carlo methods has been very brief. Monte Carlo methods have been used for solving a variety of mathematical formulations. For further details, see [18] and [19].

The list of books on simulation models in specific disciplines is very large and [20]–[25] are a small sample.

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Parameter Estimation

1 Introduction

We have used the term "parameter" in a number of ways in earlier chapters. In Chapter 3 we used it in the context of system characterization. To clearly distinguish this from others, we will designate such parameters as "system parameters". In Chapters 5 and 7 we introduced parameters in the process of developing mathematical formulations. These parameters will be called "formulation parameters". When a formulation is used to model a system, the "formulation parameters" become "model parameters".

For a given mathematical model, one needs to solve the underlying mathematical formulation to obtain the model behaviour. As indicated in Chapters 6 and 8, specific numerical values must be assigned to the model parameters to obtain the solution. The problem of finding the most appropriate values is called "parameter estimation". Different approaches must be used, depending on the nature of the underlying mathematical formulation. In this chapter we discuss methods of estimation for both deterministic and stochastic models.

2 Some Preliminaries

2.1 Notation

We shall denote by θ the unknown model parameters which need to be estimated; θ can be either a scalar or a vector. In general θ is constrained to belonging to a set Θ specified as a part of the model formulation as illustrated by the following two examples.

Example 1

Consider a model involving a time-invariant linear differential equation formulation

$$y^{(n)}(t) + \sum_{i=1}^n \alpha_i y^{(n-i)}(t) = x(t) \quad (1)$$

where $y^{(j)}(t)$ is the j th derivative of $y(t)$; $x(t)$ and $y(t)$ representing the model input and output

respectively. The parameter θ is given by an n -dimensional vector

$$\theta^T = \{\alpha_1, \alpha_2, \dots, \alpha_n\} \quad (2)$$

As a part of model formulation one might specify that bounded input must produce bounded output; in other words, the model must be stable. This is assured if the parameters are suitably constrained so as to ensure that the roots of the polynomial equation

$$P(s) = s^n + \sum_{i=1}^n \alpha_i s^{n-i} = 0 \quad (3)$$

lie in the left half-plane; i.e. they all have negative real parts. In the case $n = 1$, the constraint is given by

$$\Theta: \{\alpha > 0\} \quad (4)$$

For $n > 1$ it is given by a system of algebraic inequalities.

Example 2

Consider a model involving a stationary Markov chain formulation with two states. In this case the formulation is given by a 2×2 one-step transition matrix

$$P = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \quad (5)$$

with the constraint set Θ given by

$$\Theta = 0 \leq P_{ij} \leq 1, \quad 1 \leq i, j \leq 2, \text{ and} \\ \sum_{j=1}^2 P_{ij} = 1, \quad 1 \leq i \leq 2 \quad (6)$$

As indicated above we have four parameters – i.e.

$$\theta^T = \{P_{11}, P_{12}, P_{21}, P_{22}\} \quad (7)$$

An alternative, but equivalent, characterization is as follows:

$$P = \begin{bmatrix} P_{11} & 1 - P_{11} \\ 1 - P_{22} & P_{22} \end{bmatrix} \quad (8)$$

with

$$\theta^T = \{P_{11}, P_{22}\} \quad (9)$$

and

$$\Theta = \{0 \leq P_{ii} \leq 1, 1 \leq i \leq 2\} \quad (10)$$

The advantage of the second characterization is that it has fewer parameters, as well as fewer constraints.

We shall employ the following notation throughout this chapter:

- θ : unknown parameter,
 - θ^* : true value of θ ,
 - $\hat{\theta}$: estimate of θ obtained using the system data,
 - n : dimension of θ ,
 - y^m, x^m : model output and input respectively,
 - y^s, x^s : system output and input respectively.
- (Note y^m, x^m, y^s and x^s can be scalar or vector.)

In the case of a static system [model], $y^s, x^s[y^m, x^m]$ are variables; in the case of a dynamic system [model] $y^s, x^s[y^m, x^m]$ can be either sequences or a function

of one or more independent variables representing time and spatial coordinates.

$T[N]$: Length of data available for parameter estimation with continuous [discrete] time data.

2.2 Estimation

In many instances the model parameters are related to the system parameter on a one-to-one basis. In this case it is sometimes possible to obtain estimates for some of the model parameters by directly measuring the corresponding system parameters, as illustrated by the following example.

Example 3 Case Study D [Cont.] (Rocket Launch)

A model for the motion of the rocket was given in Section 5.4 of Chapter 5. It involved a second-order differential equation formulation. One of the model parameters is M , the coefficient of the second derivative. It represents the mass of the rocket. Thus, in this case, we can obtain the true value of M by measuring the mass of the rocket directly.

Often it is not possible to measure system parameters directly. In the case of "black box" modelling, the system parameters are not defined, and hence no such one-to-one relationship exists between the system parameters and the model parameters. In these cases the model parameters need to be estimated using the system input and output data.

A scheme for estimating parameters is called an *estimator* and the values obtained are called *estimates*.

2.3 System Data

The system data (available for parameter estimation) are given by the observed values of the input and output variables in the case of a static system, and by their time histories in the case of dynamic systems. The data available are often less than complete, and in many instances contaminated by external factors, as illustrated by the following example.

Example 4

Suppose that the changes in the system are occurring continuously in time. In this case complete data would correspond to measuring the variables continuously in time. Often it is not possible to do this. Suppose the variables are measured using a sampling scheme which records the values at discrete time instants. In this case, instead of complete data we have only partial data, as some information is lost due to sampling. Since a variable is measured using some physical device (sensor), the measured value will differ from the true value due to what is commonly termed "measurement noise" (or error) which affects the measurement. If the magnitude of this error is small in relation to the magnitude of the variable being measured, then it can be ignored and the measurement can be viewed as being nearly accurate. If not, the effect of this error must be taken into account and the data treated as inaccurate.

The method for estimation depends on type and quality of data available for estimation.

2.4 Deterministic vs Stochastic

In deterministic systems there is no uncertainty. Unfortunately, systems are seldom deterministic, but if the uncertainty is small then it can be ignored and the system can be viewed as a deterministic system and modelled adequately by a deterministic formulation. In this case the model parameters can be obtained using a relatively small length of data, and the estimates can be viewed as being deterministic.

In stochastic systems the system variables change in an unpredictable manner. As a consequence an estimate based on finite length of data is also random. It can be characterized either through a probability distribution function or in terms of its moments. As the data length increases, the estimates might or might not converge in some probabilistic sense. If the estimates converge to the true value as the data length approaches infinity, then the estimates are said to be a consistent estimate and the estimator a consistent estimator. The convergence can be one of many types – e.g. convergence in probability, convergence in mean square or convergence with probability one. Convergence in mean square sense implies that as the data length approaches infinity, the mean of the estimate equals the true value and the variances of the estimate go to zero.

A variety of estimators has been developed for estimating the parameters of different types of stochastic models. An estimator is said to be unbiased if the mean of the estimate equals the true value. Obviously, the estimator with the smallest variance is the most desirable. For the case where the data length is sufficiently large, the maximum likelihood estimator has this property. We shall discuss this aspect further in a later section.

Comments

- (1) We use the term "model parameter" in the widest sense. For example, it can include the order of the formulation, as in an autoregressive moving-average time series formulation; the parameters of the distribution characterizing uncertainty in the system and/or measuring device and so on.
- (2) In Chapter 4 we discussed a model as a mathematical formulation related to a system characterization. To obtain model behaviour we dropped the association between the formulation and the system characterization. This allowed the analysis of the formulation to be carried out without the encumbrance of the system characterization. The behaviour of the model was obtained by re-establishing the relationship after the analysis was completed. We employ a similar approach here. As such, when we use the term model, we refer to the underlying mathematical formulation and ignore the relationship with the system characterization. Hence, estimating model parameters is really treated as estimating the parameters of the underlying formulation.

3 Deterministic Model Parameter Estimation

In Chapter 5 we discussed a variety of mathematical formulations suited for use as deterministic models. Although the structures of the formulations vary considerably, the approaches to parameter estimation are nearly the same for all. The two basic approaches to parameter estimation are:

- (1) equation error approach, and
- (2) output error approach.

In this section we commence with a restatement of some of the model formulations discussed in Chapter 5. This is followed by a brief discussion of data aspects in estimation. The equation error and output error approaches are then discussed.

3.1 Restatement of Formulations

We use the notation mentioned in the previous section – i.e. x represents the input and y the output.

A representative static model is given by

$$y^m = f(x^m, \theta) \quad (11)$$

and the data available for estimating the parameter θ are assumed to be given by

$$\{x_i^s, y_i^s\}, \quad 1 \leq i \leq N \quad (12)$$

A representative discrete time dynamic model is given by

$$y_t^m = g(\Delta[y_t^m], \Delta[x_t^m], \theta) \quad (13)$$

where

$$[\Delta z_t]_n = \{z_{t-1}, z_{t-2}, \dots, z_{t-n}\} \quad (14)$$

and the data available for estimating the parameter θ are assumed to be given by

$$\{x_t^s, y_t^s\}, \quad 1 \leq t \leq T \quad (15)$$

If x_t^s and/or y_t^s is missing for some values of t , in the interval $1 \leq t \leq T$, then we have incomplete data.

Similarly, a representative continuous time dynamic model involving ordinary differential equation formulation is given by

$$g(D[y^m(t)], D[x^m(t)], \theta) = 0 \quad (16)$$

where

$$D[z(t)]_n = \{z(t), z^{(1)}(t), z^{(2)}(t), \dots, z^{(n)}(t)\} \quad (17)$$

and

$$z^{(i)}(t) = d^i z(t)/dt^i, \quad i \geq 0 \quad (18)$$

The data available for estimating the parameter are given by

$$\{y^s(t), x^s(t)\}, \quad 0 \leq t \leq T \quad (19)$$

If the data available for estimation are given by

$$\{y^s(t), x^s(t)\}, \quad t = t_1, t_2, \dots, t_N \quad (20)$$

instead of (19), then we have reduced data as opposed to complete data. The reduction is due to sampling.

We assume that θ is an n -dimensional vector and constrained to satisfy $\theta \in \Theta$, a specified set of constraints.

3.2 Equation Error Approach

The method is shown schematically in Figure 10.1. The observed values of x^s and y^s are substituted in place of x^m and y^m in the model formulation (given by (11) for static model; (13) for discrete time dynamic model and (16) for continuous time dynamic model). As a result, the formulation can be viewed as an algebraic equation with θ being the only unknown. If the number of algebraic equations so created equals n , then these can be solved to yield an estimate $\hat{\theta}$.

When the data available are large, then the number of algebraic equations resulting from the above-mentioned substitution is greater than n . If the model is a true representation of the system, the set of algebraic equations form a set of consistent equations – i.e. solving any n equations will yield the same estimate $\hat{\theta} = \theta^*$. However, a model is only a simplified representation of the system. As a result the set of algebraic equations do not form a set of consistent equations. In other words we have an overdetermined set of inconsistent equations. In this case the estimate $\hat{\theta}$ is obtained by a least-squares approach which minimizes the sum of the square of errors in the set of algebraic equations.

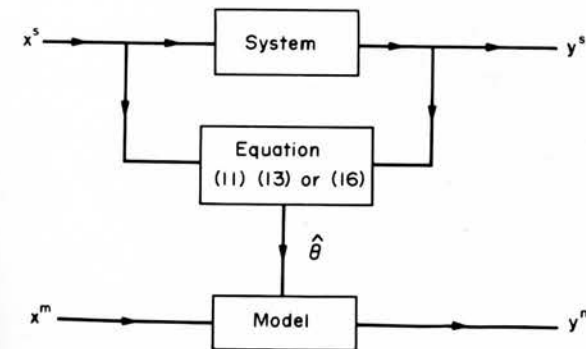


FIGURE 10.1 Equation error approach.

A major drawback of the approach for estimating continuous time dynamic model parameters is that it requires differentiating the system data. This is not desirable as often the data are contaminated with sensor noise which gets amplified under the operation of differentiation. An alternative method suitable for continuous time linear dynamic models, and not requiring any differentiation of the data, will be discussed in Section 3.4.

3.3 Output Error Approach

The method is shown schematically in Figure 10.2. In this approach the model response (i.e. y^m) is obtained for $\theta = \tilde{\theta}$ using $x^m = x^s$. Let $e(\tilde{\theta})$ denote the error between the model output and the system output - i.e.

$$e(\tilde{\theta}) = e_t(\tilde{\theta}) = y_t^s - y_t^m, \quad 1 \leq t \leq N \quad (21)$$

in the case of discrete time model, and

$$e(\tilde{\theta}) = e(t, \tilde{\theta}) = y^s(t) - y^m(t), \quad 0 \leq t \leq T \quad (22)$$

in the case of continuous time model.

Based on $e(\tilde{\theta})$, we evaluate a function $J(\tilde{\theta})$ given by

$$J(\tilde{\theta}) = \sum_{i=1}^n \{e_i(\tilde{\theta})\}^2 / N \quad (23)$$

in the case of discrete time model, and

$$J(\tilde{\theta}) = \int_0^T \{e(t, \tilde{\theta})\}_2^2 dt / T \quad (24)$$

in the case of continuous time model.

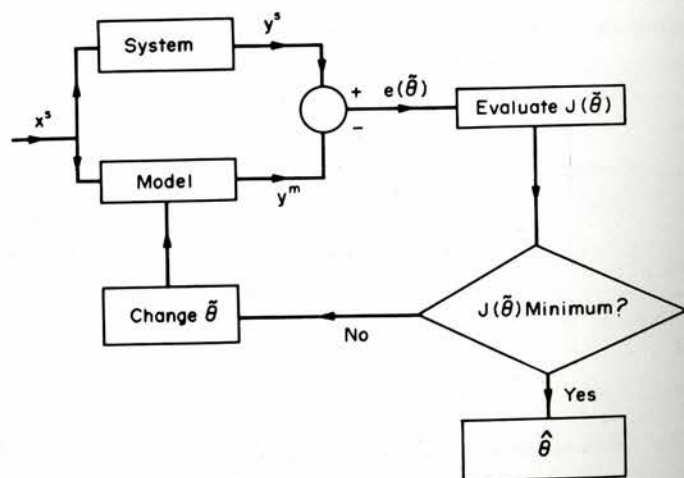


FIGURE 10.2 Output error approach.

$J(\tilde{\theta})$ is an indicator of the misfit between the system and the model outputs with the model parameter $\theta = \tilde{\theta}$. The estimate $\hat{\theta}$ is the value of θ which minimizes $J(\theta)$. It can be obtained by using one of many iterative schemes available for function minimization subject to constraints, as θ is constrained to belong to Θ .

3.4 Special Method for Linear Dynamic Model

This method is applicable only for models involving linear ordinary differential equation formulations with time-invariant parameters. The parameters of the model are the coefficients of the differential equation. If the model input be

$$x^m(t) = \sin(\omega t) \quad (25)$$

then the output under steady state conditions is given by

$$y^m(t) = A^m(\omega, \theta) \sin(\omega t + \phi(\omega, \theta)) \quad (26)$$

where $A^m(\omega, \theta)$ and $\phi(\omega, \theta)$ are functions of the frequency ω and model parameter θ . (They are called "gain" and "phase" respectively.) By selecting $x^s(t) = x^m(t)$ as given by (25) we can experimentally measure the resulting system output $y^s(t)$ and hence obtain the system gain $A^s(\omega)$. Equating the model gain with the system gain - i.e.

$$A^s(\omega) = A^m(\omega, \theta) \quad (27)$$

we have an algebraic equation with θ being the unknown. By obtaining $A^s(\omega)$ for different values of ω , we have n algebraic equations which can be solved to yield an estimate $\hat{\theta}$. We illustrate by a simple example.

Example 5 (First-order Model)

The model is given by

$$dy^m(t)/dt = ay^m(t) + bx^m(t) \quad (28)$$

with the parameter θ and the constraint Θ given by

$$\theta = \{a, b\}, \quad \Theta = \{a < 0, b \neq 0\} \quad (29)$$

Using $x^m(t)$ given by (25) we have

$$A^m(\omega, \theta) = b / \sqrt{a^2 + \omega^2} \quad (30)$$

Thus, by experimentally evaluating $A^s(\omega)$ for two different values of ω , and using (27) with $A^m(\omega, \theta)$ given by (30), we can solve for a and b . Note that the solution yields two values for a - one negative and one positive. The negative is the one to be accepted as the positive violates the model parameter constraint given by (29).

3.5 Case Study A [Cont.] (Weight Lifting)

In Section 3.2 of Chapter 5 we discussed various models for relating the weight lifted (L) to the body weight (W). In this section we consider estimating model parameters for Models A.2 and A.3.

MODEL A.2

The model is given by

$$L = kW^{2/3} \quad (31)$$

with θ and Θ given by

$$\theta = \{k\}, \quad \Theta = \{k > 0\} \quad (32)$$

Using the data given in Table 2.2 and the equation error approach, we have

$$\hat{k} = 18.49 \quad (33)$$

MODEL A.3

The model is given by

$$L = k(W - W_0)^\beta \quad (34)$$

with θ and Θ given by

$$\theta = \{k, W_0, \beta\}, \quad \Theta = \{k > 0, W_0 > 0, \beta > 0\}. \quad (35)$$

We assume $W_0 = 30$. Then, using the data given in Table 2.2 and the equation error approach, we have the following estimates:

$$\hat{k} = 64.256, \quad \hat{\beta} = 0.44335. \quad (36)$$

3.6 Case Study E [Cont.] (World Population)

In Section 5.5 of Chapter 5 we discussed a variety of models for the evolution of $N(t)$, the total population at time t . In this section we consider estimating the model parameters for Model E.5.

MODEL E.5

The model is given by

$$dN(t)/dt = f(N(t), \theta)N(t) \quad (37)$$

We consider a specific form for f as indicated below:

$$f(N(t), \theta) = a(L - N(t)) \quad (38)$$

with the parameters and the constraints given by

$$\theta = \{a, L\}, \quad \Theta = \{L > 0\} \quad (39)$$

We assume a value for L and estimate a using the output error approach and the data given in Table 2.3. The estimated values are as follows.

- (i) $L = 15 \times 10^9$ $\hat{a} = 2.307 \times 10^{-3}$
 - (ii) $L = 20 \times 10^9$ $\hat{a} = 1.722 \times 10^{-3}$.
- (40)

4 Stochastic Model Parameter Estimation

In Chapter 6 we discussed a variety of formulations suited for use as stochastic models. A number of methods have been developed for estimating stochastic model parameters. Some of the methods are applicable for all types of models whilst others are applicable to specific models. In this section we discuss the three commonly used methods. They are:

- (i) method of least squares;
- (ii) method of moments; and
- (iii) method of maximum likelihood.

We employ the notation defined in Section 2 and the standard convention of using upper-case letters to represent random variables and lower-case letters to represent their outcomes or realized values.

4.1 Method of Least Squares

The method of least squares is ideally suited for estimating parameters of regression models. As indicated in Section 4.3 of Chapter 7, a regression model is of the form

$$Y_i^m = g(x_i^m, \theta) + V_i^m \quad (41)$$

where V_i^m is an unknown random variable with zero mean and finite variance. Y_i is random due to V_i^m being random.

Let the system data available for estimating θ be given by

$$(x_i^s, y_i^s), \quad 1 \leq i \leq N \quad (42)$$

(Note: y_i^s is the realized outcome of Y_i^s which is random due to uncertainty in the system.)

The estimate $\hat{\theta}$ is obtained by minimizing $J(\theta)$ given by

$$J(\theta) = \sum_{i=1}^N \{y_i^s - g(x_i^s, \theta)\}^2 / N \quad (43)$$

i.e. $\hat{\theta}$ is the value of θ which yields a minimum value for $J(\theta)$. Note that the parameters are obtained by viewing y_i^s as a realization or outcome of the model with $x_i^m = x_i^s$. Because y_i^s is a random outcome, the estimate $\hat{\theta}$ is a random variable. If the sequence $\{V_i\}$ is an independent sequence, then as $N \rightarrow \infty$, $\hat{\theta} \rightarrow \theta^*$ in probabilistic sense as defined in Section 2.4.

The method of least squares is also suited for estimating deterministic model parameters when the observations are contaminated with sensor noise. We shall assume that the noise is additive. As a result the sensor output Y_0^s is related to the true output y^s by a relation

$$Y_0^s = y^s + V \quad (44)$$

where V is an independent stochastic process with zero mean and finite variance representing the sensor noise.

The error between the observed output y_0^s and the model output is given by

$$e(\tilde{\theta}) = y_0^s - y^m \quad (45)$$

Since y_0^s is an outcome of the random variable Y_0^s , minimizing the sum of error squares using $J(\tilde{\theta})$ as defined by (23) or (24) yields an estimate $\hat{\theta}$, which is random, and converges to the true value θ^* as $N \rightarrow \infty$. However, $J(\theta)$ does not go to zero as $N \rightarrow \infty$. It approaches a limit σ^2 , the variance of the sensor noises.

If the uncertain term V in (41) or (45) is correlated (as opposed to being statistically independent) then the estimate $\hat{\theta}$ might not converge to θ^* as $N \rightarrow \infty$. In this case the method has to be suitably modified to take the correlation into account.

4.2 Case Study J [Cont.] (Speed of Aeroplanes)

In Section 4.4 of Chapter 7 we proposed three stochastic models involving regression formulations for this problem. In this section we consider estimating parameters for Models J.1 and J.2(b).

MODEL J.1

The model is given by

$$Y^m(t) = a_1 + b_1(t - 1900) + V^m(t) \quad (46)$$

with

$$\theta = \{a_1, b_1\} \quad (47)$$

Using the method of least squares and the system data, for the period 1900–1940, given in Table 2.6, we have the following estimates:

$$\hat{a}_1 = 47.07, \quad \hat{b}_1 = 11.35 \quad (48)$$

MODEL J.2 (b)

The model is given by

$$\log Y^m(t) = a_3 + b_3(t - 1900) + V^m(t) \quad (49)$$

with

$$\theta = \{a_3, b_3\} \quad (50)$$

The estimates using the method of least squares and the above-mentioned data are as follows.

$$\hat{a}_3 = 3.75, \quad \hat{b}_3 = 0.053 \quad (51)$$

4.3 Change in Notation

We depart from our earlier convention where we used superscript m to indicate model variables – e.g. Y^m and y^m referred to the random output and its realized

value. Henceforth we shall drop the superscripting for model variables and use Y and y in place of Y^m and y^m . However, we shall continue to use superscript s for the system variables, as in the past.

4.4 Method of Moments

In the method of moment the parameters are obtained by the following three-step procedure.

Step 1: Obtain expressions for the moments of Y in terms of the model parameters. Let M_j , the j th moment of Y , be related to the model parameters θ by the function $g_j(\theta)$, i.e.

$$M_j = E[Y^j] = g_j(\theta), \quad j \geq 1 \quad (52)$$

Step 2: Obtain estimates of M_j using the system data available. Let the available data be given by

$$\{y_i^s\}, \quad 1 \leq i \leq N \quad (53)$$

Then the estimate $\hat{M}_j$ can be obtained as follows.

$$\hat{M}_j = \sum_{i=1}^N \{y_i^s\}^j / N \quad (54)$$

Step 3: Obtain $\hat{\theta}$ by solving (52) with $\hat{M}_j$ used instead of M_j , i.e. by solving the equation

$$g_j(\hat{\theta}) = \hat{M}_j, \quad 1 \leq j \leq n \quad (55)$$

The method yields consistent estimates if $\hat{M}_j$ converge to the true M_j as $N \rightarrow \infty$.

In the case of stationary stochastic process formulation one needs moments involving the variable at two different time instants. For example, one might use

$$v_j = E[Y_i Y_{i+j}] = h_j(\theta) \quad (56)$$

in the case of discrete time formulation, or

$$v(\tau) = E[Y(t)Y(t+\tau)] = h(\tau) \quad (57)$$

in the case of continuous time formulation. The estimates for v_j and $v(\tau)$ are given by

$$\hat{v}_j = \sum_{i=1}^{N-j} (y_i^s y_{i+j}^s) / (N-j) \quad (58)$$

and

$$\hat{v}(\tau) = \int_0^{T-\tau} \{y^s(t)y^s(t+\tau)\} dt / (T-\tau) \quad (59)$$

As the data length available for estimation (i.e. T or N) $\rightarrow \infty$ the estimate $\hat{\theta} \rightarrow \theta^*$ if $\hat{y}_j$ and $\hat{v}(\tau)$ converge to the true values y_j and $v(\tau)$ respectively.

Note that, as in the previous method, the parameters are estimated by viewing the system output as a realization of the model output.

4.5 Case Study I [Cont.] (Component Reliability)

In Section 6.7 of Chapter 7 we proposed two models for modelling the time to failure. In this section we will obtain estimates of the parameters for Model I.1.

MODEL I.1

Let the time to failure (or equivalently, the age at failure) for the i th control element be Y_i . We assume that Y_i , $1 \leq i \leq n$ is a sequence of independent and identically distributed random variables with a distribution function $F(y, \lambda)$ given by

$$F(y, \lambda) = 1 - e^{-y/\lambda} \quad (60)$$

In this case the parameter to be estimated, and the constraint, are given by

$$\theta = \{\lambda\}; \quad \Theta = \{\lambda \geq 0\} \quad (61)$$

Since θ is a scalar, we need to obtain an expression for one moment only. We shall use the first moment M_1 , which is given by

$$M_1(\lambda) = E\{Y\} = \lambda \quad (62)$$

Using the data given in Table 2.5, from (52) we have

$$\hat{M}_1 = 1.561 \quad (63)$$

Using $M_1(\lambda) = \hat{M}_1$, we have the estimate $\hat{\lambda}$ given by

$$\hat{\lambda} = 1.561 \quad (64)$$

4.6 Method of Maximum Likelihood

Let $f(y_1, y_2, \dots, y_N; \theta)$ represent the joint density function for the set of random variables $(Y_1, Y_2, \dots, Y_N)$ of the model under consideration. Let y_i , $1 \leq i \leq N$, be the observed (or realized) values of Y_i . The likelihood function expresses the likelihood of this set of values being the outcome, and can be written as

$$L(\theta) = L(y_1, \dots, y_N; \theta) = f(y_1, y_2, \dots, y_N; \theta) \quad (65)$$

Given y_i , $1 \leq i \leq N$, and the model structure, the only unknown in L is θ , the parameters to be estimated.

In the method of maximum likelihood the estimate $\hat{\theta}$ is obtained by

maximizing $L(\theta)$ given by (65) with y_i , $1 \leq i \leq N$, being replaced by the corresponding system data y_i^s . In other words, $\hat{\theta}$ is the model parameter which maximizes the likelihood of the observed data, y_i^s , $1 \leq i \leq N$, being the random outcome (or realization) of the model.

$\hat{\theta}$ can be obtained either by maximizing $L(\theta)$ directly or by solving the set of equations given by

$$\partial L(\theta) / \partial \theta = 0 \quad (66)$$

For a given system data (i.e. y_i^s , $1 \leq i \leq N$), the $\hat{\theta}$ which maximizes $L(\theta)$ also maximizes $\log L(\theta)$, as the logarithmic transformation is monotonic. In some cases it is simpler to deal with $\log L(\theta)$ instead of $L(\theta)$.

The maximum likelihood estimate has some very desirable and interesting asymptotic properties which are as follows:

- (i) $\hat{\theta}$ is asymptotically unbiased;
- (ii) the covariance of $\hat{\theta}$ is given by

$$\text{cov}(\hat{\theta}) = M^{-1} \quad (67)$$

where

$$M = M(\theta^*) = E[\{\partial \log L(\theta) / \partial \theta\}^T \{\partial \log L(\theta) / \partial \theta\}]|_{\theta=\theta^*} \quad (68)$$

and the expectation is done over the observed random variables. $M(\theta^*)$ is called the Fischer information matrix and will be used in the next chapter;

- (iii) $\hat{\theta}$ is normally distributed with mean equal to θ^* and covariance as given in (ii);
- (iv) no other estimate has covariance smaller than M^{-1} . In other words, the maximum likelihood estimator is the most efficient estimator.

The form for $L(\theta)$ depends on the model formulation and the data available for estimation, as illustrated by the following examples.

4.7 Case Study I [Cont.] (Component Reliability)

We discussed the estimation of parameter for Model I.1 in Section 4.5, where we considered the method of moments. In this section we discuss the method of maximum likelihood.

Since the failure times Y_i , $1 \leq i \leq N$, are a sequence of independent and identically distributed random variables with a distribution function given by (60), we have the likelihood function $L(\lambda)$ given by

$$\begin{aligned} L(\lambda) &= \prod_{i=1}^N f(y_i, \lambda) \\ &= \sum_{i=1}^N (1/\lambda)^N \exp \left\{ - \sum_{i=1}^N y_i / \lambda \right\} \end{aligned} \quad (69)$$

The maximum likelihood estimate, $\hat{\lambda}$, is given by the λ which maximizes $L(\lambda)$ with

$$y_i = y_i^s, \quad 1 \leq i \leq N.$$

Rather than deal with $L(\lambda)$ we shall consider its logarithmic transformation. As such, we have from (69)

$$\log L(\lambda) = -N \log \lambda - \sum_{i=1}^N (y_i^s)/\lambda \quad (70)$$

where we have replaced y_i by y_i^s . $\hat{\lambda}$ is obtained by solving

$$d\{\log L(\lambda)\}/d\lambda = 0 \quad (71)$$

which yields

$$\hat{\lambda} = \sum_{i=1}^N y_i^s / N \quad (72)$$

Using the data from Table 2.5, we have

$$\hat{\lambda} = 1.561 \quad (73)$$

Note that for this model the estimate obtained by the method of maximum likelihood is the same as that obtained by the method of moments. In general, this is not the case.

4.8 Case Study G [Cont.] (Weather Changes)

In Section 5.3 of Chapter 7 we proposed a model (Model G.1) involving a stationary Markov chain formulation with three states for modelling the changes in weather. In this section we consider parameter estimation for this model.

MODEL G.1

This model is given by a one-step transition matrix P , which is as follows:

$$P = \begin{bmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{bmatrix} \quad (74)$$

with

$$\theta = \{P_{ij}, 1 \leq i, j \leq 3\} \quad (75)$$

and

$$\Theta = \{0 \leq P_{ij} \leq 1 \text{ for } 1 \leq i, j \leq 3, \text{ and } \sum_{i=1}^3 P_{ij} = 1 \text{ for } 1 \leq j \leq 3\} \quad (76)$$

The variable Y_t can assume only one of following three values: 1, if day t is

sunny; 2, if partly sunny – and 3, if cloudy. The system data – the realized values y_t^s , $1 \leq t \leq 63$; are as given in Table 2.4.

The above situation corresponds to complete data being available. Let n_{ij}^s ($1 \leq i, j \leq 3$) be the number of transitions from state i to j over the interval of 63 days. Then, from the data given in Table 2.4, we have n_{ij}^s given by

$$\begin{bmatrix} 18 & 9 & 5 \\ 9 & 1 & 6 \\ 6 & 5 & 3 \end{bmatrix} \quad (77)$$

with the element in the i th row and j th column representing n_{ij}^s .

To obtain the maximum likelihood estimate we need to obtain the joint distribution function for $\{N_{ij}, 1 \leq i, j \leq 3\}$, where N_{ij} represents the number of times the state has changed from i to j over the interval of 63 days. We omit the details of the derivation and present the final form of the estimator. The estimates are given by

$$\hat{P}_{ij} = n_{ij}^s / n_i^s \quad (78)$$

for $1 \leq i, j \leq 3$ and where

$$n_i^s = \sum_{j=1}^3 n_{ij}^s \quad (79)$$

Using the values given in (77) we have the maximum likelihood estimate $\hat{P}$ of P given by

$$\hat{P} = \begin{bmatrix} 18/32 & 9/32 & 5/32 \\ 9/16 & 1/16 & 6/16 \\ 6/14 & 5/14 & 3/14 \end{bmatrix} \quad (80)$$

Note that the estimates satisfy the constraints given by (76).

4.9 Case Study L [Cont.] (Demand for Soft Drinks)

In Section 7.4 of Chapter 7 we proposed a model (Model L.1) involving autoregressive moving-average formulation for predicting the demand for soft drinks. In this section we outline the method of maximum likelihood to obtain the model parameters.

MODEL L.1

The model is given by equation (53) of Chapter 7 and is reproduced below.

$$Y_t = \sum_{j=1}^n \alpha_j Y_{t-j} + \sum_{j=1}^m \beta_j W_{t-j} + W_t \quad (81)$$

with

$$\theta = \{\alpha_j, 1 \leq j \leq n; \beta_j, 1 \leq j \leq m; \sigma^2\} \quad (82)$$

and

$$\Theta = \{\text{roots of } P(s) = 0 \text{ and } Q(s) = 0 \text{ lie inside the unit circle}\} \quad (83)$$

where

$$P(s) = s^n - \sum_{j=1}^n \alpha_j s^{n-j} \quad (84)$$

$$Q(s) = s^m + \sum_{j=1}^m \beta_j s^{m-j}$$

The system data available for estimation are given by

$$\{y_t^s\}, \quad 1 \leq t \leq N. \quad (85)$$

Recall that $W_t, t \geq 1$ is a sequence of independent and identically distributed random Gaussian variables with mean zero and variance σ^2 .

Since $Y_t, t \geq 1$ is Gaussian, the joint density function for $(Y_1, \dots, Y_N)$ can be obtained but is a complicated function of θ . An approximate maximum likelihood estimate, $\hat{\theta}$, is obtained by minimizing:

$$J(\theta) = \sum_{k=n+1}^N \{\hat{w}_k\}^2 / (N-n) \quad (86)$$

where $\hat{w}_k$ is generated by the relation

$$\hat{w}_k = y_k^s - \sum_{i=1}^n \alpha_i y_{k-i}^s - \sum_{j=1}^m \beta_j \hat{w}_{k-j} \quad (87)$$

where $\hat{w}_k = 0, 1 \leq k \leq n$. The error between the true and the approximate estimates is of the order $(1/N)$ and is insignificant for large N . The estimate $\hat{\sigma}^2$ is given by the minimum value for J .

The above minimization requires an iterative computational scheme where changes to the parameters must be done in a manner so as to ensure that the constraints imposed by (83) are not violated. We examine parameter estimation in ARMA models in detail in Chapter 16.

5 Concluding Remarks

As mentioned earlier, we have confined our attention in this chapter to the three most common methods of parameter estimation for stochastic models. Many other methods have been developed which are described in the literature. Specific details are given in the Notes that follow.

Notes and References

Items [1]–[3] comprise a small sample of the large number of books on parameter estimation in general. Most books on econometrics (e.g. [4]) and on regression modelling (e.g. [5] and [6]) deal with parameter estimation for regression formulations.

Methods for estimating dynamic model parameters can be found in [7]–[15]. In general, discrete time formulations have received more attention than continuous time formulations. Items [16]–[19] list a small sample of books which deal with special methods for discrete time formulations. For more on the equation error approach, see [20]. Parameter estimation for distributed systems (i.e. systems modelled by partial differential equations) can be found in [21]–[23].

We commented briefly on sensor noise affecting observed values. Sometimes this is also called measurement error. For more on the analysis of measurement errors, see [24].

As indicated in the previous section, we have omitted various methods for estimation. For further details on the method of quasi-linearization, see [25]; on stochastic approximation, see [26]; item [27] is an illustrative sample of books on robust statistical methods. In the text we mentioned some of the interesting and desirable asymptotic properties of maximum likelihood estimators. For discussion on small sample properties, see [28].

Often the data available are incomplete. For more on estimation with missing data see [29].

There are a large number of books devoted to estimating parameters for either a particular type of model formulation (e.g. [30]) or models from specific areas of application (e.g. [31]). The *Proceedings* of the IFAC Symposium on Identification and Parameter Estimation, held every third year since 1967, contain a large number of interesting articles dealing with parameter estimation for dynamic models.

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CHAPTER 11

Design of Experiment

1 Introduction

As discussed in Chapter 3, the first step in modelling is system characterization. This requires an understanding of the system under consideration. If the system has been studied in the past, and the model builder has inherited this understanding, then very little new information is needed to execute the first step in the modelling process. If this is not the case, then the model builder must first gain a satisfactory understanding of the system before the modelling process can commence. This understanding can often be achieved through experimentation. There are other instances where experimentation is necessary; for example to provide information about the system to permit estimation of model parameters as discussed in Chapter 10 or, ultimately, to validate the model.

Experiments must be designed to yield relevant information. Optimal designs maximize the information obtained. The design of experiments depends on the type of information being sought and the reason for seeking that information. Thus, the design of experiment to improve understanding of causal relationships (needed for system characterization) will be different from those needed for estimating model parameters or validation. Since information is obtained by measuring one or more variables using sensors, often the information obtained is contaminated by sensor noise. Consequently, care must be taken in interpreting experimental results to avoid incorrect inferences.

In most real-life situations the experiment must be done under one or more constraints. The constraints can be either technical or economic. Experimental design must take these constraints into account. Often a trade-off must be sought between the quality of information obtained and the time (or cost) required to obtain it. These make the design of experiment an interesting and challenging topic.

In this chapter we focus our attention on the design of experiments to obtain additional information about the system under consideration. We start with those that provide information helpful in characterizing systems. We consider designs for static systems in Section 2 and for dynamic systems

in Section 3. Following this, we discuss optimal designs for parameter estimation. This is done in Section 4 for static systems and in Section 5 for dynamic systems. In Section 6 we discuss a topic called "response surface design", which can be thought of as the combination of experimental design and optimization. Finally, we consider the design of experiments in a bigger framework involving additional features such as the time needed for experimentation, cost factors, quality of information etc.

2 Design of Experiments for Static Systems (Causal Relationships)

Suppose the model builder has identified N variables, $X_i (1 \leq i \leq N)$, and wants to establish which of them influence some other variables Y significantly. In other words, the aim is to find out which of the N variables, $X_i (1 \leq i \leq N)$, are related to Y through a cause-effect relationship.

In the literature on design of experiments, the variables $X_i (1 \leq i \leq N)$ are called controlled factors. The reason for the terminology is that the experimenter can control them in some sense – i.e. in the selection of either the variables or the value assigned to them. Other variables which influence Y but which are not under the control of the experimenter are called uncontrollable factors.

The controllable factors are categorized as either

- (a) *qualitative* – if they assume only discrete values;
- (b) *quantitative* – if they assume a continuous range of values.

An example of the first type are the factors in Case Study B (Alloy Selection) discussed in Chapter 3, Section 6.2, where the two factors are (i) the variations in ore quality (denoted by MA) and (ii) the method of manufacture (denoted by ME). Since there are four different ore types and two different methods of manufacture, the values assigned to the two factors are given by the set $\{MA_i; 1 \leq i \leq 4 \text{ and } ME_j; 1 \leq j \leq 2\}$. Here the factors represent qualitative (categorical) features of the system under consideration. Examples of the second type can be found in most chemical, physical and engineering sciences. An example from chemical engineering is as follows. X_1 and X_2 represent the temperature and pressure at which some reaction is allowed to take place, and Y represents the percentage yield resulting from the reaction. Here, X_1 and X_2 can assume a continuous range of values and the experiment is to obtain information so that X_1 and X_2 can be selected optimally to maximize the percentage yield. We shall discuss this type of experiment in Section 6.

2.1 Experimental Design for Qualitative Factors

As mentioned earlier, in the case of qualitative factors, each controllable factor can only assume values from a finite set. The values are sometimes called levels,

indicating the origin of this chapter topic in agricultural sciences. In an experiment the experimenter can assign different values (or levels)* for each of the controllable factors. Let the levels that can be assigned to factor $X_i (1 \leq i \leq N)$ be given by the set

$$\{X_i^j, 1 \leq j < n_i\}$$

Consider an experiment to establish whether the controllable factors $X_i (1 \leq i \leq N)$ have significant influence or not on Y , which is as follows. Study the effect on Y by varying one factor, say X_k , with all other factors (i.e. $X_i, 1 \leq i \leq N, i \neq k$) held fixed. If Y does not change significantly, then we infer that X_k does not have a significant effect on Y . This approach is called the "single-factor approach" as we consider one factor at a time. This approach can lead to wrong inferences, as illustrated by the following example.

Example 1

Consider a problem in which there are two factors, i.e. $N = 2$. Let Y_{ijk} be the observed value of Y with $X_1 = X_1^i$ and $X_2 = X_2^j$ at the k th replication. Suppose that the relationship is given by

$$Y_{ijk} = (RC)_{ij} + V_{ijk} \quad (1)$$

with $(RC)_{ij} = 0$ for the following two cases

Case 1: $i = i^*, j$ arbitrary

Case 2: $j = j^*, i$ arbitrary.

$(RC)_{ij}$ is non-zero for all other combinations, and V_{ijk} is an independent Gaussian random variable with zero mean and variance σ^2 .

Suppose that the single-factor approach is used with X_1 set to $X_1^{i^*}$ and X_2 varied. This will result in the inference that X_2 has no effect on Y . Continuing the experiment with X_2 set to $X_2^{j^*}$ and X_1 varied will also result in a similar inference. The inference drawn from the experiment is obviously incorrect.

The reason for the erroneous inference in this example is that the single-factor approach yields incomplete information about the system, since all combinations of factor levels are not studied. Caution must be exercised to avoid falling into such traps.

2.2 Factorial Design

In factorial design, Y is observed for all possible combinations of factor levels. Since X_i has n_i different levels, the total number of combinations, NC , is given by

$$NC = \prod_{i=1}^N n_i \quad (2)$$

Each combination is called a cell – a term that once again reflects the origin of this topic in agricultural science.

*We shall henceforth use the term "level" instead of "value", so as to be consistent with the usage in the design of experiment.

For the two-factor case (i.e. $N = 2$) let Y_{ij} represent the observed value of Y with $X_1 = X_1^i$ and $X_2 = X_2^j$. Then, the observed values of a factorial design experiment can be represented as a 2×2 matrix, shown in Table 11.1. If the experiment involves repeated trials for each cell (i.e. a particular combination of factor levels) we employ a third subscript k . Thus, with this notation, Y_{ijk} represents the observed value of Y with $X_1 = X_1^i$ and $X_2 = X_2^j$ at the k th repeat. If there is no replication, then the subscript k is omitted.

The advantage of factorial design is that it allows for testing various types of interaction between factors. In the case of N factors the first-order interactions are of the form $X_i X_j$ (i.e. both factors appearing together); the second-order interaction are of the form $X_i X_j X_m$, and so on. By an analysis of the observed values of Y one can draw inferences whether one or more of the controllable factors have a significant influence on Y or not. This is done by a statistical test procedure which tests a null hypothesis that a factor X_i has no influence at all levels with an alternative hypothesis that it has influence at one or more levels. Analysis of variance is one such method for testing.

2.3 Analysis of Variance

We shall briefly outline the basis of the method and the construction of an Analysis Of Variance (ANOVA) table for carrying out the test. We shall confine our discussion to the two-factor case – i.e. $N = 2$, where the outcome of the experiment can be represented in tabular manner as indicated in Table 11.1.

The underlying basis of the analysis of variance was briefly discussed in Section 4.1 of Chapter 7. In the parametric model formulation the effect of X_1 and X_2 on Y is modelled by an algebraic equation formulation. It could be of the form

$$Y_{ijk} = A + R_i + C_j + V_{ijk} \quad (3)$$

or

$$Y_{ijk} = A + R_i + C_j + (RC)_{ij} + V_{ijk} \quad (4)$$

TABLE 11.1 Observed Outcome for Two-factor Factorial Design Experiment

		Factor X_2				
		X_2^1	X_2^2	...	$X_2^{n_2}$	
Factor X_1	X_1^1	Y_{11}	Y_{12}			Y_{1n_2}
	X_1^2					
	$\vdots$					
	X_1^i	...				Y_{ij}
	$\vdots$					
	$X_1^{n_1}$	Y_{n_1}				$Y_{n_1 n_2}$

where the set of parameters $\{A; R_i, 1 \leq i \leq n_1; C_j, 1 \leq j \leq n_2; (RC)_{ij}, 1 \leq i \leq n_1 \text{ and } 1 \leq j \leq n_2\}$ are interpreted as follows

- A : the overall average;
- R_i : the average deviation in A due to i th level of factor X_1 ;
- C_j : the average deviation in A due to j th level of factor X_2 ;
- $(RC)_{ij}$: the average deviation in A due to interaction between the i th level of factor X_1 and j th level of factor X_2 .

Since R_i , C_j and $(RC)_{ij}$ are average deviations from the overall average, they are constrained by the following constraints:

$$\sum_{i=1}^{n_1} R_i = 0 \quad (5)$$

$$\sum_{j=1}^{n_2} C_j = 0 \quad (6)$$

$$\sum_{j=1}^{n_2} (RC)_{ij} = 0 \quad 1 \leq i \leq n_1 \quad (7)$$

and

$$\sum_{i=1}^{n_1} (RC)_{ij} = 0 \quad 1 \leq j \leq n_2 \quad (8)$$

Note that if the relationship is given by (3), and if $R_i = 0, 1 \leq i \leq n$, then X_1 has no influence on Y . Thus in this case the null hypothesis

$$R_1 = R_2 = \dots = R_{n_1} = 0 \quad (9)$$

is to be tested against an alternative hypothesis that one or more of the R_i values are non-zero. Also note that in (3) we assume there is no interaction between X_1 and X_2 , whilst in (4) we allow for such interaction through the parameter $(RC)_{ij}$.

The term V_{ijk} is called the residual term, and represents the effect of uncontrollable (also sometimes called unassignable) factors. We assume that V_{ijk} is an independent Gaussian variable with zero mean and variance σ^2 . As a result, Y_{ijk} is also Gaussian; the sums of mean squares and the ratios of the sums of mean squares are distributed according to χ^2 and F -distributions respectively. The degrees of freedom for these distributions are functions of n_1 , n_2 and the number of replications. Thus, testing of alternative hypotheses can be done using tables for F -distribution.

2.4 Case Study B [Cont.] (Alloy Selection)

In Section 4.2 of Chapter 7 we formulated a model to study the influence of ore from different mines and the method of manufacture on the thermal coefficient of titanium alloy. The model (given by equation (9) of Chapter 7)

TABLE 11.2 Observed Values of Thermal Coefficient of Expansion for Case Study B

Mine ore	Method	
	ME ₁	ME ₂
MA ₁	5.78	5.46
	5.28	5.79
MA ₂	4.84	5.73
	6.28	4.36
MA ₃	6.82	5.76
	6.77	4.31
MA ₄	5.57	5.30
	6.44	4.86

is identical to (3) with Y_{ijk} corresponding to TC_{ijk} with factors X_1 and X_2 representing mine ore and method of manufacture respectively. As a result, we have $n_1 = 4$ and $n_2 = 2$. The data available to Alpha Inc. are the test results of two specimens (or samples) for each combination of mine ore and the method of manufacture – i.e. $k = 2$. Thus, in this case Y_{ijk} represents the thermal coefficient of expansion for the k th ($1 \leq k \leq 2$) replication obtained from a combination of ore from mine i ($1 \leq i \leq 4$) and method j ($1 \leq j \leq 2$). The test results are given in Table 11.2.

To carry out the analysis we construct the ANOVA table. For the general case it is given in Table 11.3, where the standard convention is used, i.e. when a subscript is replaced by a “.”, it corresponds to taking an average over that factor.

TABLE 11.3 ANOVA Table for Two-factor Case

Source	Degrees of freedom	Sum of squares
Between rows	$(n_1 - 1)$	$K n_2 \sum_{i=1}^{n_1} (\bar{Y}_{i..} - \bar{Y}_{...})^2$
Between columns	$(n_2 - 1)$	$K n_1 \sum_{j=1}^{n_2} (\bar{Y}_{.j.} - \bar{Y}_{...})^2$
Interactions (row $\times$ column)	$(n_1 - 1)(n_2 - 1)$	$K \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \delta^2$
Residuals (within cells)	$n_1 n_2 (K - 1)$	$\sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \sum_{k=1}^K (Y_{ijk} - \bar{Y}_{ij.})^2$
Total	$n_1 n_2 (K - 1)$	$\sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \sum_{k=1}^K (Y_{ijk} - \bar{Y}_{...})^2$

$$\delta = (\bar{Y}_{ij.} - \bar{Y}_{i..} - \bar{Y}_{.j.} + \bar{Y}_{...})$$

TABLE 11.4 ANOVA Table for Case Study B

Source	Sum of squares	D.F.	Mean squares
Mine/ore (MA)	0.7623	3	0.2541
Method (ME)	2.4103	1	2.4103
Interaction (MA–ME)	1.8171	3	0.6057
Residuals	3.6825	8	0.4603
Total	8.6722	15	

Thus,

$$\bar{Y}_{ij.} = \sum_{k=1}^K Y_{ijk}/K \quad (10)$$

$$\bar{Y}_{.j.} = \sum_{i=1}^{n_1} \sum_{k=1}^K Y_{ijk}/K n_1 \quad (11)$$

and so on.

The ANOVA table using the measured values of Y from Table 11.2 is shown in Table 11.4. To test for significance, each of the mean squares is tested against the mean square of residuals. In the case of the first factor (i.e. mine ore) the ratio of the mean square to the mean square of the residual (i.e. $0.2541/0.4603$) equals 0.55. Since the ratio is less than one, we see that the factor is not significant. In other words, the variations from mine to mine are not significant. Similarly, in the case of the second factor (i.e. method of manufacture) the ratio of the mean square to the mean square of residuals (i.e. $2.4103/0.4603$) equals 5.24. This ratio is distributed according to a F -distribution with (1, 8) degrees of freedom. Since $F_{1,8,0.95} = 5.32$, we see that the effect of the method of manufacture is just below the 5 per cent level of significance. The interaction between the method of manufacture and the mine ore is also not significant as the ratio of the mean squares (i.e. $0.6057/0.4603$) equals 1.32.

Since there appears to be a difference in the thermal coefficient of expansion between the two methods of manufacture, we need to examine the means and estimates of their standard deviations. Using the test results from Table 11.2 we have the following result:

	ME ₁	ME ₂
Mean	4.97	4.20

and the estimated standard error is given by 0.24 (i.e. $\sqrt{0.4603/8}$).

As a consequence, Alpha Inc. must choose Method 2 and reject Method 1. It does not matter which mine ore is selected.

2.5 Other Designs

The factorial design with N variables, $X_1, \dots, X_N$, and X_i having n_i levels ($1 \leq i \leq N$) requires a total of NC cells with NC given by (2). This is a large number if N and the various n_i are large. If three or more factors are considered to be independent, and their interaction is of no interest, then the factorial design can be modified to require fewer cells and hence fewer observations of Y .

Latin square and Graeco-Latin square are two of the several designs which require far fewer cells than the factorial design.

3 Design of Experiments for Dynamic Systems (Causal Relationships)

We confine our attention to stochastic dynamic systems. Let $X(t)$ and $Y(t)$ be two variables, and the aim to find whether they are related by a causal relationship. More specifically, we want to test whether $X(t)$ has any effect on $Y(t)$.

In order to devise a test one needs a proper definition for causality in a stochastic framework. For the case where t assumes discrete values (i.e. a discrete time dynamic system) Granger [33] provided a definition for X to cause Y in terms of the predictability of Y .

Let $\{A(t): t = 0, \pm 1, \pm 2, \dots\}$ be the given information including at least $\{X(t), Y(t)\}$. Let

$$\bar{A}(t) = \{A(s) | s < t\} \quad (12)$$

and

$$\bar{\bar{A}}(t) = \{A(s) | s \leq t\} \quad (13)$$

and similarly define $\bar{X}(t)$, $\bar{\bar{X}}(t)$, $\bar{Y}(t)$ and $\bar{\bar{Y}}(t)$. Let $P\{Y(t)|B\}$ denote the minimum mean square single-step predictor of $Y(t)$ given an information set B and let $\sigma^2\{Y(t)|B\}$ be the resulting mean square error (m.s.e.). Then Granger's definitions are as follows.

(i) $X(t)$ causes $Y(t)$, if

$$\sigma^2\{Y(t)|\bar{A}(t)\} < \sigma^2\{Y(t)|\bar{A}(t) - \bar{X}(t)\} \quad (14)$$

(ii) $X(t)$ causes $Y(t)$ instantaneously if

$$\sigma^2\{Y(t)|\bar{A}(t), \bar{\bar{X}}(t)\} < \sigma^2\{Y(t)|\bar{A}(t)\}. \quad (15)$$

In other words, (i) implies that if X causes Y then knowledge of $\bar{X}(t)$ reduces the uncertainty in the prediction of $Y(t)$. Similarly, (ii) implies that knowledge of $X(t)$ reduces the uncertainty in the prediction of $Y(t)$ because of the instantaneous causal relationship.

We can use the above definition for continuous time by using a predictor τ time units ahead ($\tau > 0$) in place of single step in the above definition.

Various tests have been developed for empirical detection of causality in discrete time systems based on the above definition and used extensively in modelling social and economic systems.

4 Design of Experiments for Static Systems (Parameter Estimation)

In Section 4.3 of Chapter 7 we studied regression models. The structure of a general regression model is given by an algebraic equation of the form

$$Y_i = g(X_i, \theta) + V_i \quad (16)$$

where X_i is a known input, V_i is an unknown random input and Y_i is a random output. In Chapter 10 we studied methods for estimating the parameter θ given $\{(y_i, X_i), 1 \leq i \leq N\}$ where y_i is the observed value of Y_i . The estimate $\hat{\theta}$ is a function of the observed data and since the y values are realized values of the random variable Y , the estimate is itself a random variable. The variance of the estimate depends on the method used and the input X_i , $1 \leq i \leq N$. This suggests then that the X_i values can be selected optimally so as to minimize the variance of the estimate in some sense. The selection of X_i , $1 \leq i \leq N$ to minimize the variance is called "optimal design", and in this section we examine this topic.

We commence with a model formulation in which θ appears linearly in $g(X, \theta)$; i.e. $g(X, \theta)$ is of the form

$$g(X, \theta) = h(X)\theta \quad (17)$$

We introduce various criteria for optimal design. Following this, we study the optimal design for the general case.

We initially assume that V_i , $i \geq 1$, is a sequence of independent and identically distributed Gaussian random variables with zero mean and finite variance, and that θ is a p -dimensional vector. We assume that X is a m -dimensional vector and Y can be either scalar or vector.

4.1 Linear Model

In this case the estimate $\hat{\theta}$ obtained by the method of least squares is given by

$$\hat{\theta} = (H^T H)^{-1} (H^T y) \quad (18)$$

where

$$H = \begin{bmatrix} h(X_1) \\ h(X_2) \\ \vdots \\ h(X_N) \end{bmatrix} \quad (19)$$

$$y^T = [y_1^T, \dots, y_N^T] \quad (20)$$

It is easily seen that:

$$E[\hat{\theta}] = \theta^* \quad (21)$$

and

$$\text{cov}[\hat{\theta}] = \sigma^2 (H^T H)^{-1} \quad (22)$$

Since $\{V_i\}$ is an uncorrelated Gaussian sequence the estimate obtained by the method of maximum likelihood is also the same. In other words $\hat{\theta}$ given by (18) is the minimum variance estimator. Note that the covariance of $\hat{\theta}$ is a function of $X_1, X_2, \dots, X_N$.

4.2 Optimality Criteria

As the covariance of $\hat{\theta}$ depends on X_i , $1 \leq i \leq N$, it suggests that a good experimental design is one that makes this matrix small in some sense. Since there is no unique ordering of the $p \times p$ matrix $(H^T H)^{-1}$, various real-valued functions have been suggested as measures of "smallness" for defining the optimality criteria. Some of the well-known ones are as follows.

(i) *D-Optimality* – A design is said to be *D-optimal* if it minimizes

$$D = |(H^T H)^{-1}| \quad (23)$$

i.e. D is the determinant of the covariance matrix.

(ii) *A-Optimality* – A design is said to be *A-optimal* if it minimizes

$$A = \text{tr} \{ (H^T H)^{-1} \} \quad (24)$$

where tr is the trace operator.

(iii) *E-Optimality* – A design is said to be *E-optimal* if it minimizes the maximal eigenvalue of $(H^T H)^{-1}$.

The minimization is done with respect to X_i , $1 \leq i \leq N$, and X_i being constrained to belonging to some region $\bar{X}$, a subset of R^m if X is a m -dimensional vector. Thus the optimal design is reduced to a constrained function optimization problem. In general, a computational iterative scheme would be needed to obtain the optimal design.

Note that, for the linear model, the optimal X_i^* , $1 \leq i \leq N$, are independent of the parameters being estimated.

4.3 General Model

We assume that V_i , $i \geq 1$, is a sequence of independent and identically distributed random variables with a density function $f(v)$ and is not necessarily Gaussian. As a result the maximum likelihood estimate $\hat{\theta}$ is given by the value of θ which maximizes

$$L = \sum_{i=1}^N \log f(y_i - g(X_i, \theta)) \quad (25)$$

and the variance of the estimate is given by

$$\text{var} \hat{\theta} = M^{-1} \quad (26)$$

with

$$M = M(\theta^*) = E\{[\partial L / \partial \theta]^T [\partial L / \partial \theta]\}_{|\theta=\theta^*} \quad (26')$$

where the expectation is done over the observed data and θ^* is the true value of θ .

As in the earlier case, the optimal design, for estimating the parameter θ , requires choosing X_i , $1 \leq i \leq N$, to minimize a function of M . Thus the procedure is similar to the linear model case except the matrix $(H^T H)^{-1}$ is replaced by the matrix $M(\theta^*)$. Note that if the sequence V_i , $i \geq 1$, is not an independent sequence, then the log-likelihood function L is more complicated.

However, in contrast to the linear model case, the optimal X_i^* , $1 \leq i \leq N$, are a function of θ^* – the unknown true values of the parameter. This is rather awkward as the experiment is to obtain information for estimating the unknown parameter, but the design requires knowledge of this unknown quantity.

One way of overcoming this situation is to model the initial (or prior) knowledge of θ^* by a distribution function, and consider M given by

$$M = E\{M(\theta^*)\} \quad (27)$$

where the expectation is done over θ^* .

5 Design of Experiments for Dynamic Systems (Parameter Estimation)

The philosophy for optimal design of experiments to estimate parameters of dynamic system models is similar to that for static system models. We shall confine our discussion to models involving either ordinary differential equation or difference equation formulations. If the uncertainty in the system is insignificant and the variables are measured accurately (i.e. the sensor noise is insignificant) then the estimation problem is relatively straightforward and the design of experiment not difficult. The design of experiment becomes significant, as well as interesting, when there is uncertainty either in the system and/or in the measuring device, so that the observed system output variables must be viewed as realizations of a stochastic process.

In Section 4.6 of Chapter 10 we discussed the method of maximum likelihood for stochastic models. As indicated there, for large data lengths, the maximum likelihood estimate is the most efficient estimate – i.e. no other estimate has smaller variance. The covariance of the maximum likelihood estimate $\hat{\theta}$ is given by the Cramer–Rao inequality, i.e.

$$\text{cov}(\hat{\theta}) = M^{-1} \quad (28)$$

where M is the Fischer information matrix given by

$$M = E[\{\partial L([Y]; [x]; \theta)/\partial \theta\}^T \{\partial L([Y]; [x]; \theta)/\partial \theta\}]|_{\theta=\theta^*} \quad (29)$$

where Y is the system output, x is the system input and $[Y]$ and $[x]$ are given by

$$\begin{cases} [Y] = Y(t), & 0 \leq t \leq T \\ [x] = x(t), & 0 \leq t \leq T \end{cases} \quad (30)$$

in the case of continuous time model, and by

$$\begin{cases} [Y] = Y_n, & 0 \leq t \leq N \\ [x] = x_n, & 0 \leq t \leq N \end{cases} \quad (31)$$

in the case of discrete time model. The expectation is done over $[Y]$ and θ^* is the true value of θ .

Thus, in this case, we see that the variance of the estimate $\hat{\theta}$ is a function of the input $[x]$. In optimal design of experiment the input $[x]$ is chosen so as to make the variance of the estimate small in some sense.

5.1 Input Constraints

Often the input that can be used in experimentation must be constrained due to physical reasons. For example, if the absolute magnitude cannot exceed a level A , then we have the constraint

$$|x^i(t)| \leq A, \quad 1 \leq i \leq m \quad (32)$$

in the case of continuous time system and

$$|x_i^j| \leq A, \quad 1 \leq i \leq m \quad (33)$$

in the case of discrete time system. We have assumed that the input x is a m -dimensional vector and x^i represents the i th component of x .

In the case of continuous time system $\{x^T(t)x(t)\}$ represents the input power at time t . Hence, if the experiment be done for a period $0 \leq t \leq T$, then the total energy used is given by

$$\int_0^T \{x^T(t)x(t)\} dt \quad (34)$$

Often the total energy available is limited, and this gets translated into the constraint

$$\int_0^T \{x^T(t)x(t)\} dt \leq \alpha \quad (35)$$

For the case of discrete time systems we have the energy constraint given by

$$\sum_{i=1}^T x_i^T x_i \leq \alpha \quad (36)$$

The optimal design of experiment must take into account such constraints if they are relevant.

5.2 Optimality Criteria

If θ is a p -dimensional vector, the covariance of $\hat{\theta}$, given by (28), is a $p \times p$ matrix. We need to define a suitable criterion to compare different designs and for selecting the optimal. As in the case of static system, a variety of criteria have been proposed – the more popular ones being the A -optimality and the D -optimality. The two are similar to that defined in Section 4.2, and hence will not be repeated here.

We illustrate by a simple example involving a first-order differential equation model.

Example 2

Suppose that the system is adequately modelled by the formulation

$$\tau dy(t)/dt = -y(t) + x(t) \quad (37)$$

with τ being the unknown parameter with τ^* its true value. The input $x(t)$ is restricted to being sinusoidal, i.e.

$$x(t) = \sin(\omega t) \quad (38)$$

with ω being the free parameter which the designer must choose optimally.

We assume that the output of the sensor $Y_o(t)$ is related to the system output $y(t)$ by the relation

$$Y_o(t) = y(t) + V(t) \quad (39)$$

with $V(t)$ being a Weiner process with zero mean and unit variance. Note that $V(t)$ represents the sensor noise. The observed output is given by $y_o(t)$, $0 \leq t \leq T$.

Let the criterion for selecting the optimal ω^* be given by

$$\phi(\bar{M}) = -\log |\bar{M}| \quad (40)$$

where $\bar{M}$ is the average information per unit time, i.e.

$$\bar{M} = M/T \quad (41)$$

with M given by (29). Since there is only one parameter (i.e. $p = 1$), the Fischer information matrix is a scalar and is given by

$$M = T2\omega^2 / \{1 + (\omega\tau^*)^2\}^2 \quad (42)$$

(The details of the derivation have been omitted, and can be found in the reference cited in the Notes at the end of the chapter.)

As a result, using (42) and (41) in (40), we have

$$\phi(\bar{M}) = -\log [2\omega^2 / \{1 + (\omega\tau^*)^2\}] \quad (43)$$

The optimal ω^* is obtained by solving the equation

$$\partial \phi(\bar{M}) / \partial \omega = 0 \quad (44)$$

which yields

$$\omega^* = 1/\tau^* \quad (45)$$

Note that the optimal frequency is a function of the true value of the parameter which is unknown.

Thus, as in the case of static system, the optimal design suffers from the drawback that it is a function of the true value of the parameter – a quantity

which is unknown. This is rather awkward as the goal of the experiment is to estimate this unknown. Various approaches have been proposed to overcome this drawback, and we discussed one such in Section 4.3.

5.3 Optimal Sampling

In continuous time systems the system variables change continuously with time. Often, measuring these variables continuously in time is not practical. In some instances (e.g. for processing the data on digital computer) one needs only sampled values of continuous variables.

When sampling is employed, the sampling strategy becomes a part of the design of the experiment. We shall confine our attention to uniform sampling – i.e. the variables are sampled at time instants $t = k\Delta$, $k = 0, 1, 2, \dots$; Δ is called the sampling interval which the experimenter must choose carefully.

In general, sampling implies a certain loss of information from the signal being sampled. However, if the signal is band limited to $[-f, f]$, then a uniform sampling at a rate $f_s \geq 2f$ will result in no loss of information as the original signal can be reconstructed from the sampled values. This result is useful in the context of designing optimal input and sampling schemes for estimating parameters of linear dynamic models.

If the system is adequately modelled by a deterministic linear time-invariant ordinary differential equation, then the output $y(t)$ resulting from sinusoidal input $x(t)$ (given by (38)) is of the form

$$y(t) = A(\omega) \sin(\omega t + \phi(\omega)) \quad (46)$$

i.e. the output is also a sinusoidal signal of the same frequency but differing in both amplitude and phase. Thus, using a sampling scheme with sampling rate $f_s = \omega/\pi$ (i.e. $f_s = 2f$) will imply no loss in information.

The data available for estimation are the sampled values contaminated with sensor noise. The optimal design is obtained in the manner described earlier – i.e. optimizing a suitable optimality criterion involving the Fischer information matrix obtained from the likelihood function of the sampled values of the variables. We illustrate by considering the model of Example 2.

Example 3

The model is as given in Example 2, and the parameter to be estimated is τ . We impose the constraint that $x(t)$ is of the form given by (38), as a result of which $y(t)$ is of the form given by (46). We employ a sampling rate

$$f_s = 2f = \omega/\pi \quad (47)$$

The average information per unit observation is given by

$$\bar{M} = 2\pi\omega / \{1 + (\omega\tau^*)^2\}^2 \quad (48)$$

(The details of the derivation have been omitted, and can be found in the reference cited in the Notes at the end of the chapter.) Using the criterion given by (40), we have the optimal ω^* given by

$$\omega^* = 1/(\sqrt{3}\tau^*) \quad (49)$$

and the optimal sampling rate

$$f_s^* = \omega^*/\pi = 1/(\sqrt{3}\pi\tau^*) \quad (50)$$

or

$$\Delta^* = \sqrt{3}\pi\tau^* \quad (51)$$

Note that again the optimal design is a function of the true value of the parameter which is unknown.

5.4 Case Study H [Cont.] (Thermal Power Station)

In Section 6.8 of Chapter 3 we briefly discussed the system characterization of a thermal power station for designing regulators. The function of the regulators is to change the operating condition of the boiler, turbine and generator as the electrical load changes.

In order to design proper regulators one needs to model the relationships which link changes in input to changes in output for each of the three subsystems – viz. boiler, turbine and generator. In this section we consider only the boiler, and confine our attention to the case where the changes are small so that the relationships can be adequately modelled by ordinary linear differential equations. The model is as shown in Figure 11.1, with the input variables being the changes in the firing rate and the valve setting and the output variables being the changes in the pressure and the steam flow. Note that the approach taken in building this model is the “black-box” approach, and each of the four boxes represents linear dynamic relations. The aim of the experiment is to obtain the parameters of the linear dynamic relationships. By using an approach along the lines of Examples 2 or 3 (depending on whether

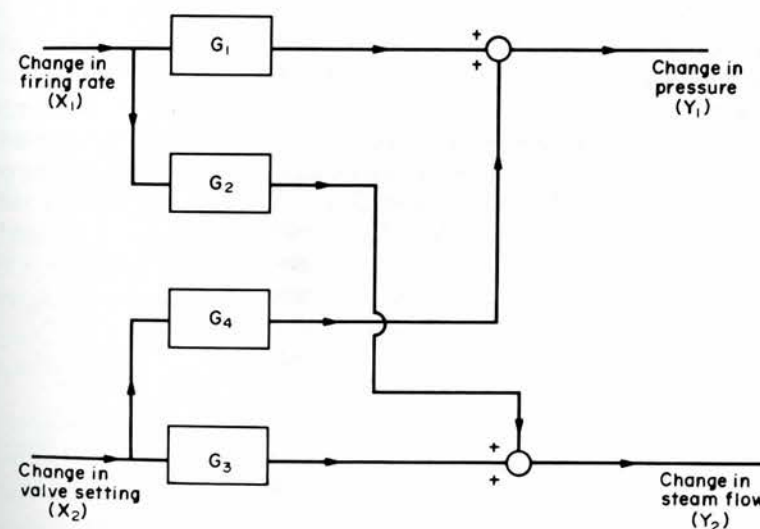


FIGURE 11.1 Model of boiler for Case Study H.

the output is measured continuously or is sampled), the input to yield optimal estimates can be found.

6 Response Surface Design

In its simplest form, response surface methodology uses simple mathematical models involving low-degree polynomial formulations to approximate the relationship between the output variable (called response variable) and a set of input variables over a range of interest. Since the input variables can assume a continuous range of values, they can be viewed as quantitative factors affecting the response variable.

The response variable represents a measure of the system performance – e.g. yield or efficiency. One of the aims of the response surface design is to improve the performance of the system by systematically varying the input variables using the measured values of the response variable. This use of the response surface methodology is known as evolutionary operation (EVOP). Various design schemes have been formulated and studied in this context.

7 Other Aspects

The discussion of the design of experiment so far has been done in a very narrow framework. The discussion has ignored features such as time and cost factors and quality of information. In this section we discuss the design of experiments which take these features into account.

7.1 Time and Cost Factors

As mentioned in Chapter 10, the variance of parameter estimate is a function of the data length used in the estimation. The larger the data length, the smaller the variance of the estimate, i.e. the variance is inversely related to data length. However, larger data length implies experimentation over a longer period of time. Since experimentation involves human and material resources, the cost of an experiment increases with the duration of the experiment. Thus a suitable trade-off must be made between the variance of the estimate and the cost of experimentation. This is achieved by defining a suitable criterion which incorporates the cost aspect as well as the quality of the estimate. A fairly general form for such a criterion is given by

$$J = g(c, T, N) + \phi(M) \quad (52)$$

where $\phi(M)$ is a measure of the quality of the estimate and g is a measure of the cost of experimentation. The parameters c, T, N and M have the following meanings:

c = cost of experimentation per unit time,

T = total time period for experiment,

N = number of points sampled if a sampling scheme be used, and

M = Fischer information matrix.

The function g is an increasing function of its arguments and the function ϕ decreases as the variance of the estimate decreases. Thus, in this case, the optimal experiment is the one which yields a minimum value for J . The trade-off is highly problem-dependent, as illustrated by the following two examples.

Example 4 (Introducing New Brand)

Suppose that a manufacturer of detergents is planning to introduce a new brand so as to increase his market share. A Markov chain formulation can be used to model the change in the market share with the release of the new brand. The entries of the one-step transition matrix would characterize the probability of switching between brands. The economic viability of introducing the new brand would depend crucially on the parameters of the one-step transition matrix.

To obtain data for estimating the parameter, the manufacturer might decide to do some field trials. In this case he has to decide on what population size he should have in his field trial, and the number of weeks that he should carry out the trial. The larger the value for both these variables, the better is the quality of the data for estimating parameters. But this implies greater cost of experimentation. Thus, in this case, the manufacturer must decide on a suitable trade-off between cost of experimentation and quality of data obtained.

Example 5 (Oil Drilling)

Oil drilling is a costly and risky venture. Geological survey yields some data but is not very reliable. A more refined experimentation is the use of seismic exploration. This is more expensive but gives better-quality information about the presence of oil. Drilling sample holes is still more expensive but yields definite results regarding the presence of oil. Thus, in this case, the oil explorer must decide on how to spend his total exploration budget optimally so as to maximize the probability of finding oil, given that he can select different types of experimentation and that he has a choice of more than one site. This is a good example of the trade-off between cost and quality of information in experimentation.

We end this chapter by considering the design of an experiment for Case Study I.

7.2 Case Study I [Cont.] (Component Reliability)

In Section 4.5 of Chapter 10 we examined the estimation of the parameters of the distribution function for the time to failure. There we assumed that the failure data were given. When no failure data are available, the data must be obtained by experimentation. In this section we propose a variety of schemes for experimentation.

SCHEME 1

Select N components and put them into operation on a test bench which simulates the working environment for the component. The experiment is stopped after a pre-specified time period T . Let K represent the number of

elements that fail during the experiment. This is a random variable assuming integer values in the interval $[0, N]$. The data available for estimation are given by x_i , $1 \leq i \leq K$, the ages at failure for the K failed components and the additional information that $(N - K)$ components have survived for a period of T .

SCHEME 2

Select N components and put them into operation on a test bench as in Scheme 1. The experiment is stopped at the instant when the n th failure occurs, where n is a pre-specified number. Thus, in this case, the time interval for the experimentation is a random variable. The data available for estimation are given by x_i , $1 \leq i \leq n$, the ages at failure for the n failed components and the additional information that the remaining $(N - n)$ components have survived till τ given by

$$\tau = \max \{x_i, 1 \leq i \leq n\} \quad (53)$$

In both these schemes the experimenter has to select N , the number of components to put on the test bench. In Scheme 1 the duration of experiment is fixed, whilst in Scheme 2 it is a random variable. The cost of experimentation under Scheme 1 is

$$d[E(K)] + cT \quad (54)$$

and under Scheme 2 it is

$$dn + cE[\tau] \quad (55)$$

where d is the cost associated with the failure of a component and c is the cost of conducting the experiment per unit time. These costs have to be traded against the quality of the estimate obtained using the data from the experiment.

SCHEME 3 (Accelerated Testing)

If the mean time to failure is large, then under Scheme 1 we might have $K = 0$ if T is small, and under Scheme 2 τ becoming very large. One way of reducing the time for experimentation is to subject the component to a hostile environment which will hasten (or accelerate) the time to failure. This is achieved by changing the environmental conditions – e.g. the electrical and/or mechanical stresses applied, the temperature of the environment and so on. This approach is called “accelerated testing”.

The technique is justified only when a relationship exists between the parameters of the failure distributions under normal and accelerated conditions. Various types of relationships have been advocated. The “power-law”

relationship is one such, and is given by

$$\theta = \theta_0(V/V_0)^p \quad (56)$$

where θ is the model parameter under a stress level V and θ_0 is the value under the normal stress level V_0 . Thus, if $V > V_0$ and $p > 1$ then $\theta > \theta_0$. If the mean time to failure is inversely related to θ then increasing V implies a shorter time period for completing the test.

Notes and References

Design of experiments for static models have been studied for a long time and a large number of books are available on the topic. Items [1]–[8] are a small sample. In addition, there are many books on specific designs (e.g. [9]) or design of experiments for specific model formulations (e.g. [10]). The case where some data are missing is discussed in [11]. For more on optimal design, see [12]–[14].

In contrast to static models, the design of experiments for dynamic models has received attention only over the past 15 years. For more on design of experiments for models involving difference or ordinary differential equations, see [15]–[18]. Most of the new results can only be found either in journals or conference proceedings – e.g. [19] deals with the design of experiments for distributed systems (i.e. systems involving partial differential equation formulations).

The detailed derivation of the results of Examples 2 and 3 can be found in [18].

Application of experimental designs for either understanding or parameter estimation in different disciplines has also received a lot of attention as seen through the large number of books that have appeared; [20]–[29] give an illustrative sample.

For more on response surface methodology, see [30]–[32].

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CHAPTER 12

Validation

1 Introduction

In Chapter 4 we defined a mathematical model as a symbolic representation involving an abstract mathematical formulation obtained by relating the mathematical formulation to a system characterization on a one-to-one basis. A mathematical model is called an adequate model if it is adequate for the purpose (or goal) in the mind of the modeller. In Chapter 1 we indicated the motivation for building mathematical models as being the desire to solve real-world problems. Thus a mathematical model is an adequate mathematical model if it captures the salient features of the system associated with the problem, and is capable of yielding a meaningful solution to the original problem.

Validation is the process of establishing the adequacy of a given mathematical model. It is the last step in the modelling process and, in some ways, the most difficult step to execute. It involves the definition of a test (or procedure) to decide whether a given model is adequate or not. If the model passes the test, then the modelling activity comes to an end and the model can be used with confidence to obtain solutions to the original problem. On the other hand, if the model fails the test, then one has to back-track and start a new iteration in the modelling process.

In this chapter we focus our attention on validation. More specifically we concentrate on whether the model is in agreement with the system it is modelling. We commence with a brief discussion on the fundamental difficulty in validation; this is done in Section 2. Following this, we discuss the different approaches to validating models in a fairly general framework in Section 3. In Section 4 we discuss tests for validating deterministic models and in Section 5 we consider the same for stochastic models. In Section 6 we consider the comparison and ranking of alternate adequate models.

2 The Fundamental Difficulty

As indicated earlier, validation involves defining a suitable test to decide whether the model is in agreement with the system in some sense determined

by the modeller. Thus, the crucial feature is the test used in validation. If the test is too stringent, then we have the following:

- (i) The modelling process will require a large number of iterations to complete the exercise. (This is based on the assumption that one starts with the simplest mathematical formulation and system characterization and progressively increases the complexity with each iteration.)
- (ii) The final model which passes the test will be too complex, and hence of limited use in solving the original problem.

On the other hand, if the test is not stringent enough, then we have the following:

- (i) Practically any model will pass the test.
- (ii) The final model can be such a poor representation that it is practically useless for solving the original problem.

This is the fundamental difficulty which makes validation the most difficult step in the modelling process. Whatever the test, the degree of stringency must achieve a suitable trade-off between the complexity of the model and the agreement between the model and the system being modelled. In modelling, one starts with a degree of stringency based on the model builder's intuition and past experience. It may well need altering during the modelling process so as to achieve a suitable trade-off of the kind discussed above. We shall discuss the degree of stringency further when we consider specific tests in later sections.

3 Approaches to Validation

The two distinctly different approaches to validation are as follows:

- Approach 1:* based on model assumptions,
- Approach 2:* based on model behaviour.

We can combine elements of the above two approaches and define a third approach:

- Approach 3:* based on model assumptions and behaviour.

We shall briefly discuss each of the above three approaches and illustrate through examples.

3.1 Approach 1 (Model Assumptions)

In this approach the inadequacy of a model is established by a critical examination of the basic assumptions made in building the model. The

justification for the approach is that if the assumptions are invalid then the agreement between the model behaviour and the system behaviour will be poor, and hence the model will not be adequate to solve the original problem. Thus, rejecting a model based on this approach saves the effort needed in the analysis, estimation, experimentation, etc., for the model.

The rejection of a model based on this approach is highly problem-dependent, as illustrated by the following example.

Example 1

A model is to be built to describe the motion of a simple pendulum. If the time interval of study is sufficiently small, so that the energy loss due to frictional drag is very small, then the assumption that the frictional drag is negligible is valid. However, if the time interval of study is large, then a model built on the assumption that the frictional drag is negligible is not valid, since the effect of drag on the pendulum motion is cumulative. Hence, in this case the model should be rejected.

In the above example, the decision to reject a model as not being adequate was based on the time interval of study and not on the actual system data – i.e. the data for pendulum motion. In some cases one either requires system data or some analysis to establish the validity of the assumptions of a model, as illustrated by the following examples.

Example 2 (Weather Changes: Case Study G)

For Case Study G (Weather Changes) we formulated three models (Models G.1 to G.3) in Section 5.3 of Chapter 7. Model G.1 assumes a Markov property for the changes in the weather. To decide whether this assumption is valid or not will require system data and a suitable statistical test.

Example 3 (Rocket Launch: Case Study D)

For Case Study D (Rocket Launch) we formulated a model (Model D.1) in Section 5.4 of Chapter 5. The assumption that the thrust is an impulse is valid if the thrust lasts for a very small fraction of the total flight time; something that is not known initially. Only after a first solution can this be checked. This again emphasizes the iterative nature of modelling.

It is important to note that valid assumptions by themselves are not sufficient to ensure the adequacy of a model. Hence, as indicated earlier, this approach is useful in establishing the “inadequacy”, rather than the “adequacy”, of a given model. In addition, this approach is of limited use in the case of models where the underlying assumptions are not stated explicitly, as with “black-box” modelling.

3.2 Approach 2 (Model Behaviour)

In this approach the validity of a model is established by a test which evaluates the agreement between model and system behaviour. *The assumptions made in model building are not important.* What matters is how close the output of the model is to the output of the system for equivalently controlled input. The closeness is determined by the stringency of the test. The test involves the error

between the model and the system outputs in the case of deterministic models, and the statistical properties of the model and the system outputs in the case of stochastic models.

Since this approach involves system data, it is desirable that the data used for validation be different from those used for estimating the model parameters, to ensure that validation is independent of parameter estimation. Typically, one should divide the available system data into two parts, with the first part (comprising the initial two-thirds of the total data) to be used for parameter estimation and the second part (comprising the final one-third of the total data) for validating the model. This is possible when the data available are sufficiently large. When the data are limited, the same data must be used for both estimation and validation.

In Sections 4 and 5 we discuss tests for validating deterministic models and stochastic models respectively.

3.3 Approach 3 (Model Assumption/Model Behaviour)

In this approach the validity of a model is established by:

- (i) checking the validity of the assumption on which the model is built, and
- (ii) the closeness of the agreement between the behaviour of the model and the system.

In other words, this approach is a combination of the two earlier approaches; it thus contains the good features of both.

4 Validation of Deterministic Models

We shall first consider models with one independent variable, i.e. models involving either ordinary differential equation or difference equation formulations. Let $y^s(t)$ and $y^m(t)$ represent the system output and the model output respectively for the same input $u(t)$. The independent variable t represents time, and assumes a continuous range of values in continuous time modelling and a discrete set of values in discrete time modelling. The actual error between the two outputs, $e(t)$, is given by

$$e(t) = y^s(t) - y^m(t) \quad (1)$$

and the relative error by

$$\tilde{e}(t) = e(t)/y^s(t) \quad (2)$$

4.1 A Test for Validation

The closeness between model and system behaviour can be defined in terms of an index J involving either the actual error $e(t)$ or the relative error $\tilde{e}(t)$ over the

time interval for which system data are available for validation. The index J characterizes the goodness-of-fit. Without loss of generality, we assume that the data available for validation are given by

$$y^s(t), \quad 0 \leq t \leq T \quad (3)$$

in the case of continuous time model and by

$$y^s(t_i), \quad 0 \leq i \leq N \quad (4)$$

in the case of discrete time model.

A simple form for J is given by

$$J = \int_0^T e^T(t)e(t)dt \quad (5)$$

or

$$J = \int_0^T \tilde{e}^T(t)\tilde{e}(t)dt \quad (6)$$

for continuous time model, and by

$$J = \sum_{i=1}^N e^T(t_i)e(t_i) \quad (7)$$

or

$$J = \sum_{i=1}^N \tilde{e}^T(t_i)\tilde{e}(t_i) \quad (8)$$

in the case of discrete time model. Other forms for J can also be used.

We accept the model as an adequate representation of the system if J is less than some pre-specified value δ . If J is bigger than δ the model is regarded as being an inadequate representation, and hence rejected.

The value assigned to δ determines the stringency of the test. As δ gets smaller, the test becomes more stringent. The value one assigns to δ is subjective, and must be based on a suitable trade-off between the goodness-of-fit and the complexity of the model.

Suppose that δ is small and that J is given by (5)–(8). Can one be sure that the test will always ensure that the model behaviour is in good agreement with the system behaviour? The answer is *NO* – as illustrated by the following example.

Example 4

Let $y^s(t)$ be the system output and $y_1^m(t)$ and $y_2^m(t)$ be the outputs of two different models (M_1 and M_2 respectively), as shown in Figure 12.1. Then using the above test with δ fairly small ($\sim 10^{-2}$) we have model M_1 pass the test whilst model M_2 fails the test. However, one should prefer M_2 to M_1 as M_2 models the significant feature (i.e. large rise and fall) whilst M_1 does not

The above example suggests that the simple form for J given by (5)–(8) is not the most appropriate for establishing the adequacy of a model. In other words, we need to use more complex forms for J .

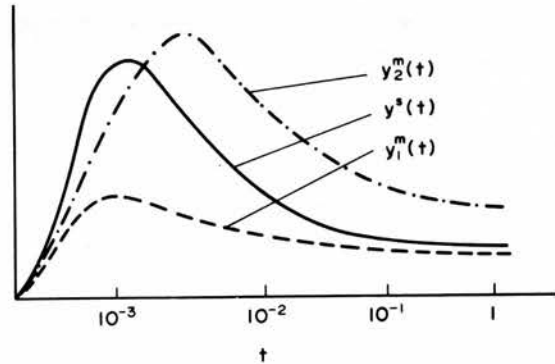


FIGURE 12.1 Plot of system and model responses for Example 4.

4.2 Characterization of Goodness-of-fit

The formulation of a suitable index J to characterize the goodness-of-fit is a non-trivial task. It must ensure that the model behaviour matches the system behaviour and reflects the salient feature of the system behaviour. The salient features could be, for example

- (i) the number of turning points in the system output;
- (ii) the maxima (or minima) of the system output and the time instants at which they occur.

Thus a more suitable index for Example 4 would be

$$J = \gamma_1 \int_0^T \{e(t)\}^2 dt + \gamma_2 |y^s(t_1^s) - y^m(t_1^m)| + \gamma_3 |t_1^m - t_1^s| \quad (9)$$

where $t_1^s[t_1^m]$ is the time instant at which $y^s(t)$ [$y^m(t)$] reaches maximum; γ_i , $1 \leq i \leq 3$, are non-negative constants reflecting the relative weights attached to the various deviations between model and system responses.

4.3 Two or More Independent Variables

In this case both the model and the system responses are functions of the independent variables (x, y, z) representing spatial coordinates, and t representing time. The goodness-of-fit index, J , must take into account the error between the two responses over the range of the independent variables. In the case of two independent variables, with the ranges given by $a \leq x \leq b$ and $0 \leq t \leq T$, two simple forms for J are as follows:

$$J = \int_a^b dx \int_0^T \{e(x, t)\}^2 dt \quad (10)$$

with $e(x, t)$, the error between the responses given by

$$e(x, t) = y^s(x, t) - y^m(x, t) \quad (11)$$

or

$$J = \sum_{i=1}^N \int_0^T \{e(x_i, t)\}^2 dt \quad (12)$$

with $a \leq x_1 < x_2 < \dots < x_N \leq b$, and the x_i , $1 \leq i \leq N$ specified.

4.4 Effect of Sensor Noise

So far we have assumed implicitly that the system output is measured accurately. In other words, there is no error in the sensor used for measuring the system output variable. Often the measured value of the system differs from the true value due to the influence of sensor noise. In this case the measured output $y_0^s(t)$ is related to the true output $y^s(t)$ by

$$y_0^s(t) = y^s(t) + V(t) \quad (13)$$

with $V(t)$ representing the sensor noise. As a result the test needs to be modified to take into account the influence of $V(t)$. Note that with sensor noise, the index J (given by (5)–(8)) is greater than zero even if $y^m(t) = y^s(t)$; i.e. the model output is identical to the true system output.

If $V(t)$ is a scaled Wiener process with a scaling factor α , $y^s(t)$ and $y^m(t)$ are scalar and J is given by (5), then

$$E[J] = \alpha^2 T + \int_0^T e^2(t) dt \quad (14)$$

where $e(t)$ is given by (1).

This suggests the following modification to the test given earlier. Accept the model if $J \leq \alpha^2 T + \delta$ and reject the model if $J > \alpha^2 T + \delta$ with $\delta > 0$. As with the earlier test, δ reflects the stringency of the test. However, this is not a good test for establishing the adequacy of a model. If T is small, then the difference between J and its expected value has high variability and hence the test can result in wrong inferences. On the other hand, if T is large, then $\alpha^2 T$ tends to dominate δ and the effect of δ is lost.

An alternative approach is to evaluate the difference between the measured system output and the model output; i.e. $y_0^s(t) - y^m(t)$, for discrete values t_i , $1 \leq i \leq I$, in the interval $[0, T]$. If $y^m(t)$ is fairly close to $y^s(t)$, then $y_0^s(t_i) - y^m(t_i)$, $1 \leq i \leq I$, is a sequence of random variables with approximately the same statistical properties as the sequence $V(t_i)$, $1 \leq i \leq I$. Since $V(t_i)$, $1 \leq i \leq I$ is a sequence of independent and identically distributed Gaussian random variables with zero mean and finite variance, the adequacy of the model can be established by a suitable statistical test involving the statistical property of the sequence $y_0^s(t_i) - y^m(t_i)$, $1 \leq i \leq I$ and comparing it with the corres-

ponding statistical property of the sequence $V(t_i)$, $1 \leq i \leq I$. We shall discuss such tests in the next section.

4.5 Case Study A [Cont.] (Weight Lifting)

In Section 3.2 of Chapter 5 we proposed three models (Models A.1 to A.3) which relate the weight lifted (L) to the body weight of the lifter (W). We considered estimating model parameters in Section 3.5 of Chapter 10 using the data given in Table 2.2.

As the data length is short, we used all the data in parameter estimation and hence there are no independent data for validation. As such, we are forced to use the same data for the purpose of validation.

We use J given by

$$J = \sum_{i=1}^N \{ [L_s(W_i) - L_m(W_i)] / L_s(W_i) \}^2 \quad (15)$$

as the index of the goodness-of-fit. $L_s(W_i)$ is the actual weight lifted by a lifter with body weight W_i and $L_m(W_i)$ is the corresponding value predicted by the model. We accept the model as being adequate if $J \leq \delta$ with $\delta = 10^{-3}$ and reject it as being inadequate if $J > \delta$.

Using the model parameters estimated in Section 3.5 of Chapter 10, the values for J for the two models are as follows.

$$\text{Model A.1} \quad J = 1.035 \times 10^{-3}$$

$$\text{Model A.2} \quad J = 0.406 \times 10^{-3}$$

Model A.1 is not an adequate model as $J > \delta$, whilst A.2 is. If δ is reduced to 10^{-4} , then we see that neither of them is an adequate model.

5 Validation of Stochastic Models

In stochastic system modelling, the data available for validation y_i^s , $1 \leq i \leq N$ are a realization (or outcome) of the system output variable Y_i^s , $1 \leq i \leq N$. Let Y_i^m , $1 \leq i \leq m$, represent the variables of the model which correspond to Y_i^s . If the model be simulated (as indicated in Chapter 9) we have a set of model outcomes y_i^m , $1 \leq i \leq N$ which can be viewed as a realization of Y_i^m .

One might be tempted to use the test of the previous section (i.e. based on the goodness-of-fit between y_i^s and y_i^m , $1 \leq i \leq N$) to validate the model. Unfortunately, this is not meaningful as the realized value of the model (i.e. y_i^m , $1 \leq i \leq N$) changes if the simulation is repeated. Thus, one needs a different approach for validating stochastic models. In this section we discuss two different approaches. *These are statistical comparison of responses and hypothesis testing.*

5.1 Statistical Comparison of Responses

Let Q_s represent some statistical characterization of the system response. It could be, for example, the probability density function or the moments of the system output. Note that Q_s is deterministic. Let Q_m represent the statistical characterization for the corresponding model response.

Since both Q_s and Q_m are deterministic, we can use the error between the two as an indicator of the mismatch between the system and the model, with the mismatch being viewed in a statistical sense.

A SIMPLE TEST FOR ESTABLISHING MODEL ADEQUACY

A simple test is as follows: define a goodness-of-fit index J as a functional of the error between Q_m and Q_s in a manner similar to that in the previous section. If $Q_s[Q_m]$ is the stationary probability density function $p_s(y)$ [$p_m(y)$] of the system [model] outputs $Y_s(t)$ [$Y_m(t)$] and the outputs are scalar, then a suitable J is given by

$$J = \int_{-\infty}^{\infty} \{ p_s(y) - p_m(y) \}^2 dy \quad (16)$$

If $Q_s[Q_m]$ are the first J moments M_s^j [M_m^j], $1 \leq j \leq J$, then a suitable J is given by

$$J = \sum_{j=1}^J \{ M_s^j - M_m^j \}^2 \quad (17)$$

As in the previous section, we accept the model as being an adequate model if $J \leq \delta$ where δ is a specified positive quantity. If $J > \delta$ then the model is rejected as being inadequate. The value of δ determines the stringency of the test.

For a given model, Q_m can be obtained by either analytical or computational methods. Unfortunately Q_s cannot be obtained in a similar manner. However, an estimate $\hat{Q}_s$ of Q_s can be obtained using the system data available for validation. Thus, the testing for adequacy is to be done using $\hat{Q}_s$ instead of Q_s . The drawback of this test is that if the data available for estimation are limited then $\hat{Q}_s$ is a poor estimate of Q_s and hence the test can lead to wrong inference.

5.2 Hypothesis Testing

In hypothesis testing we use the observed system data to test a null hypothesis against an alternative hypothesis. In the context of model validation the null hypothesis would be that the observed system data have come from the model under test (in other words, the model is an adequate representation of the system), and the alternative hypothesis would be that it has come from some other model.

The decision to accept or reject the null hypothesis is done by a test which divides the space of observations into two regions – A and B – the null hypothesis is accepted as being true if the observed data falls in region A and rejected otherwise. As a consequence, one can make two types of error:

Type I error: Rejecting the null hypothesis when it is actually true.

Type II error: Accepting the null hypothesis when it is false.

The probabilities of making these two errors depend on how the space of observations is divided. It is impossible to make both these probabilities arbitrarily small. In general, tests are designed (i.e. the division of the space of observations into two regions) such that the probability of Type I error does not exceed some pre-specified value α . This value is called the significance level of the test. The probability of Type II error be given by β ; $(1 - \beta)$ is called the power function of the test. A test in which α is fixed and $(1 - \beta)$ is maximized is called the uniformly most powerful test.

Various methods have been proposed for the division of the space of the observations. Depending on the model formulation, the decision to accept or reject can be reduced to testing a statistic involving the null hypothesis and the observed data. We shall illustrate this point by considering three specific model formulations. We omit the details of derivation, and interested readers should consult the reference cited at the end of the chapter.

5.3 Validating Markov Chain Model

Let the model be given by a Markov chain formulation with r states and the parameter of the one-step transition matrix be given by

$$P_{ij} = P_{ij}^0, \quad 1 \leq i, j \leq r \quad (18)$$

In this case the null hypothesis is that the state of the system evolves with the one-step transition matrix given by (18).

Using the system data available for validation, we obtain estimates $\hat{P}_{ij}$, and compute a statistic J given by

$$J = \sum_{i=1}^r \sum_{j=1}^r \tilde{n}_i (\hat{P}_{ij} - P_{ij}^0) / P_{ij}^0 \quad (19)$$

where $\tilde{n}_i$ is the number of times the process was in state i over the interval of the data used in the validation. Asymptotically J is distributed according to a χ^2 distribution with $(r(r-1)-d)$ degrees of freedom, where d is the number of P_{ij}^0 which are zero and the summation in (19) is done only over (i, j) for which $P_{ij}^0 > 0$.

From the tables of χ^2 distribution we evaluate $\Pr\{\chi^2 \geq J\}$ with J given by (8). We accept the model as an adequate representation if

$$\Pr\{\chi^2 \geq J\} < \alpha \quad (20)$$

for a given level of significance of α . If (20) is not satisfied, we reject the model as being adequate to represent the system.

5.4 Validating Deterministic Model with Sensor Noise

We considered the effect of sensor noise in Section 4.4. Using the notation of that section, we have the error

$$e(t) = y_o^s(t) - y^m(t) \quad (21)$$

to be approximately equal to $V(t)$ if the model is an adequate model – i.e. the model response is very close to the system response.

If $V(t)$ is a scaled Weiner process, and the model adequate, then $e(t_i)$, $1 \leq i \leq n$, is a sequence of independent and identically distributed random variables with zero mean and variance σ^2 . In this case a model can be validated by testing the null hypothesis that $e(t_i)$, $1 \leq i \leq n$, is a sequence of independent and identically distributed random variables. If σ^2 is known, then the test would involve a χ^2 distribution. If σ^2 is not known, then the test would be based on a Student distribution. As in the previous example, the acceptance or rejection of the null hypothesis will depend on the significance level.

If one does not make any assumptions about the distribution of $V(t_i)$ then non-parametric tests can be used to decide whether the null hypothesis is true or not.

5.5 Validating ARMA Model

Let the data available for parameter estimation and validation be the system output given by y_i^s , $1 \leq i \leq N + M$. We use the initial data – viz. $1 \leq i \leq N$ for parameter estimation and the remainder – viz. $N + 1 \leq i \leq N + M$ for validation.

Assume that the model is given by an ARMA formulation

$$y_t^m = \sum_{i=1}^n \alpha_i y_{t-i}^m + \sum_{i=1}^n \beta_i \omega_{t-i} + \omega_t \quad (22)$$

where the order n is specified, and the parameters estimated by the method of maximum likelihood – viz. by minimizing $\sum \hat{\omega}_t^2$ where $\hat{\omega}_t$ is given by

$$\hat{\omega}_t = y_t^s - \sum_{i=1}^n \alpha_i y_{t-i}^s - \sum_{i=1}^n \beta_i \hat{\omega}_{t-i} \quad (23)$$

The underlying assumption of ARMA formulation is that ω_t , $t \geq 0$ is an independent and identically distributed Gaussian sequence with zero mean and variance σ^2 .

We see from (22) and (23) that if the model is an adequate representation then $(\hat{\omega}_t)$ must be a sequence with statistical properties identical to that for the

$\{\omega_t\}$ sequence. Thus a test for establishing adequacy can be devised by checking for the independence of the $\{\hat{\omega}_t\}$ sequence. In other words, the null hypothesis is that the sequence $\{\hat{\omega}_t\}$ is an independent Gaussian sequence with zero mean and variance σ^2 .

Towards this end, let $\hat{R}_k$ be the k th sample autocorrelation of $\hat{\omega}_t$ obtained by

$$\hat{R}_k = \left\{ \sum_{t=n+1}^{N-k} [\hat{\omega}_t \hat{\omega}_{t+k}] / [N - k - (n+1)] \right\} / \left\{ \sum_{t=n+1}^N \hat{\omega}_t^2 / [N - (n+1)] \right\} \quad (24)$$

$1 \leq k \leq K$ and $K \ll N$. If the model is an adequate representation, then $\hat{R}_k$ is approximately Gaussian in distribution with zero mean and variance proportional to $1/N$, for $1 \leq k \leq K$. Also, $\hat{R}_1, \dots, \hat{R}_K$ are statistically independent.

Thus, a simple test for model validation is as follows: if $\hat{R}_k$, $1 \leq k \leq K$, lie in an interval $-\delta/\sqrt{N}$ to $+\delta/\sqrt{N}$, $\delta > 0$, then the null hypothesis is true and the model an adequate representation. As δ gets smaller the test becomes more stringent.

An alternative test which requires $K > n$ is as follows: compute Q by the relation

$$Q = \sum_{k=1}^K \hat{R}_k \quad (25)$$

If the model is adequate, then Q is distributed according to a χ^2 distribution with $(K - n)$ degrees of freedom. Using tables for χ^2 distribution, one can decide whether the null hypothesis is true or not, for a given significance level.

Note that the tests described so far validate the model in terms of the underlying assumptions (i.e. in the spirit of Approach 1). We combine this with a test involving system and model response – i.e. comparing $y_t^s - y_t^m$ for $N+1 \leq t \leq N+M$, then the validation is in the spirit of Approach 3.

5.6 Case Study J [Cont.] (Speed of Aeroplanes)

In Section 4.2 of Chapter 10 we discussed the problem of estimating the parameters of Models J.1 and J.2(b) for predicting the speed of aeroplanes in the year 2000. The estimation was done using the historical data (from Table 2.6) for the period 1900–1940. In this section we discuss the validation of these two models using the remaining part of the data – i.e. the data covering the period 1941–1965. This period contains 21 data points and hence we use the following criterion for the validation purpose.

Define ϕ as

$$\phi = \sum_{i=1}^{21} \{ |x_i^s - x^m(t_i)| / x_i^s \} / 21 \quad (26)$$

where t_i , $1 \leq i \leq 21$, are the time instants at which the speed changed due to technological improvements.

We accept the model as being adequate (for the purpose of forecasting) if $\phi \leq 0.05$ and reject the model if $\phi > 0.05$.

MODEL J.1

Using the parameter values of Section 4.2 of Chapter 10, the forecasts are given by

$$x^m(t) = 47.07 + 11.35(t - 1900) \quad (27)$$

A plot of the forecasts, along with the historical data is given in Figure 12.2. It is clear that $\phi > 0.05$ and hence the model must be rejected.

MODEL J.2(b)

For this model the forecasts are given by

$$x^m(t) = \exp \{ 3.75 + 0.053(t - 1900) \} \quad (28)$$

and plots of model output and historical data are given in Figure 12.3. In this case ϕ is < 0.05 and hence we can accept the model as being adequate for forecasting purposes. The forecast value for the year 2000 is 16,000 mph.

Comment. Since the model assumes an exponential growth, it is doubtful if the model can be used with credibility for long-term forecasting. For short-term forecasting the credibility is not in dispute.

MODEL J.3

We discussed this model briefly in Section 4.4 of Chapter 7. This model views changes in maximum speed as being due to improvements within a technology and due to changes in the technology. The changes in the technology are modelled by a scale factor of 5 and 15, as discussed in that section. As a result, the model for forecasting is given by (27) for $1900 \leq t \leq 1940$ by

$$x^m(t) = A + 56.75(t - 1940) \quad (29)$$

for $1940 \leq t \leq 1980$, where A is the forecast value from (27) for $t = 1940$, and by

$$x^m(t) = B + 170.25(t - 1980) \quad (30)$$

where B is the forecast value from (29) for $t = 1980$.

The forecasts from this model, along with the historical data, are shown in Figure 12.2, and in this case again we have $\phi < 0.05$, implying that the model is adequate for the purposes of forecasting. The forecast value for the year 2000 is given by 8700 mph.

Comment. This model is superior to Model J.2(b) as it characterizes the effect of change in technology more explicitly, as opposed to merely assuming an exponential growth.

We could have used alternative tests involving the residuals (i.e. difference

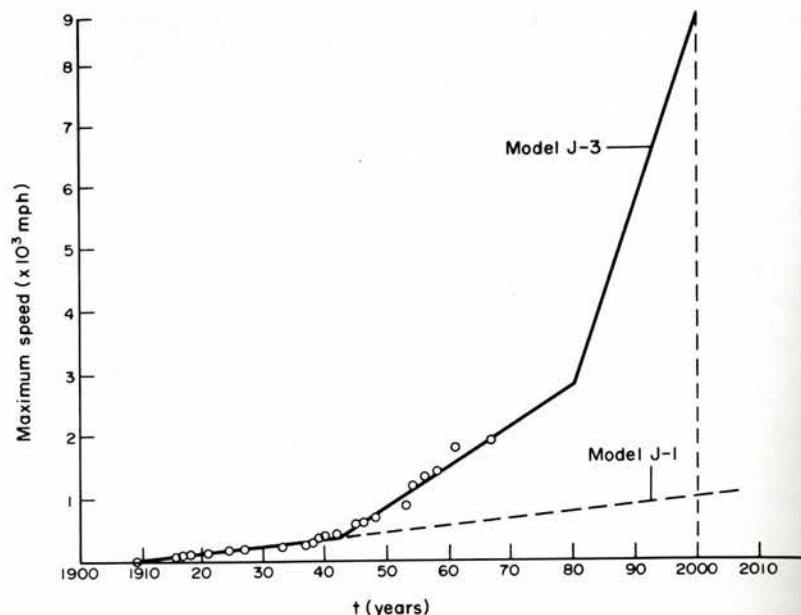


FIGURE 12.2 Forecasts, Models J.1 and J.3.

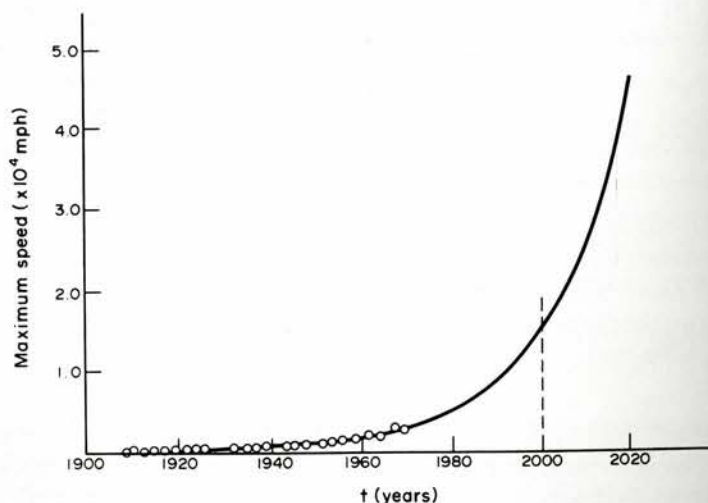


FIGURE 12.3 Forecasts, Model J.2(b).

between the data and the model predictions) since for an adequate model these would be a sequence of independent and identically distributed random variables. The test employed in this section is more in the spirit of Approach 2, whilst a test based on residuals would be in the spirit of Approach 1.

5.7 Case Study G [Cont.] (Weather Changes)

The model described in Section 5.3 of Chapter 7 for weather changes involved parameter estimation using the data given in Table 2.4. In this section we assume that the one-step transition matrix is given by the matrix

$$P^0 = \begin{bmatrix} 0.55 & 0.30 & 0.20 \\ 0.60 & 0.00 & 0.40 \\ 0.50 & 0.30 & 0.20 \end{bmatrix} \quad (31)$$

Thus, the null hypothesis is that the one-step transition matrix P is given by

$$P = P^0 \quad (32)$$

We want to test this against the alternative hypothesis that

$$P \neq P^0 \quad (33)$$

We shall assume that the data available for testing this hypothesis are the data given in Table 2.4. (Note we have estimated P^0 using some other data.)

We follow the procedure outlined in Section 5.3 and evaluate the statistics J given by (19). The $\hat{P}_{ij}$ and $\hat{n}_i$ are the same as given in Section 4.8 of Chapter 10. Using these values and that given in (31) we have

$$J = 3.3369 \quad (34)$$

If P^0 is the true one-step transition matrix, then J is distributed according to a χ^2 distribution with 5 degrees of freedom. This follows as P^0 has one zero entry. From the tables of χ^2 distribution with 5 degrees of freedom we should accept the model if $J < 1.145$ and reject the model if $J \geq 1.145$ for 5 per cent level of significance. Since $J > 1.145$, we must reject the null hypothesis and view the model as being inadequate.

6 Selection Among Alternative Models

In general, there will be more than one model that will pass the validation test. This is to be expected, for in modelling one takes a pluralistic view of the system being modelled; hence there will be more than one adequate model. Thus, given two or more different adequate models the question that arises is the following: Is one of them better than the rest in some sense? In this section we briefly discuss two factors that can be used to rank different models (for a given system) to indicate the best.

6.1 Principle of Parsimony

In this, a model M_1 is preferred to a model M_2 if M_1 has fewer parameters. Thus models can be ranked in terms of the number of parameters in the model. This type of ranking is meaningful, for the cost and effort involved in parameter estimation and design of experiment increase with the number of parameters.

6.2 Parameter Sensitivity

If a model response is highly sensitive to the parameters of the model, then the model is of limited use for prediction purposes, as small errors in parameters will result in large errors in the model response. Thus, models can be ranked in terms of the sensitivity of the response to changes in parameter values. This requires defining a suitable sensitivity index. One such is the following:

$$J(\theta) = \int_0^T \{\delta y^T(t) \delta y(t)\} dt / \{\delta \theta^T \delta \theta\} \quad (35)$$

where $\delta\theta$ is the change in θ and δy is the change in model output due to change in the parameter. (It is assumed that both θ and $y(t)$ are vectors.) The above index is one of many that can be used. Also, the ranking based on one index might not agree with the ranking with a different one.

Notes and References

Validation is in some sense the most difficult step to execute in the modelling process. In general, books on mathematical modelling contain very little discussion on the topic.

Most of the work done on model validation is scattered in various journals: [1]–[11] give a small sample; [12] and [13] examine model validation for a class of model formulations.

There are a large number of books on parametric as well as non-parametric methods for testing (e.g. [14]–[16]) which discuss various statistical tests of use in modelling. For more on hypothesis testing, see [17].

Further details of the derivation of the results of Section 3.6, see [18]. Validation methods for time series modelling can be found in a large number of books on time series modelling (e.g. [19]).

For further discussion on the role of parsimony, see [20]; on sensitivity, see [21] and [22]; and on complexity, see [23]; [24] and [25] discuss validation of models in economics.

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Pitfalls in Modelling

"A pitfall is a conceptual error into which, because of its specious plausibility, people frequently and easily fall" (Majone, 1980).

1 Introduction

Since mathematical modelling is a multi-stage activity requiring a variety of concepts and techniques, there are many pitfalls which, if not avoided, can lead the unwary modeller to produce absurd models and hence absurd solutions to the original problem which motivated the modelling exercise. In this chapter we focus our attention on these pitfalls in mathematical modelling.

2 Pitfalls

Some of the main pitfalls which the model builder should be aware of are listed below.

- (1) Forgetting that modelling is not an end in itself but is only a means towards solving real problems.
- (2) Failure to understand the problem properly and as result producing models of limited value.
- (3) Forgetting that a model is only a simplification of the real world associated with the problem, and that the two are not the same.
- (4) System characterization being not appropriate for the problem requiring solution.
- (5) Confusing correlation with causation and vice-versa in system characterization.
- (6) Using a mathematical formulation which is not well posed in a mathematical sense.
- (7) Failure to check the validity of simplification and/or the correctness of the use of mathematical techniques.
- (8) Failure to recognize the ill-conditioned nature of the formulation in the case of solving ill-conditioned formulations on computer.
- (9) Using inconsistent estimators for parameter estimation.

- (10) Poor or incorrect design of experiment which yields little new or relevant information.
- (11) Failure to interpret properly the results of mathematical analysis in physical terms of the problem.
- (12) Poor selection of criterion for validation.
- (13) Failure to critically evaluate the limitations of the model and the credibility that one should attach to the solutions obtained.
- (14) Forcing the problem to fit a particular model rather than choosing the most appropriate model for the problem.
- (15) Failure to achieve sensible compromise between conflicting factors.
- (16) Forgetting that the aim is to produce the simplest adequate mathematical model.
- (17) Failure to recognize one's own limitation. For complex problems, one needs people with different backgrounds to build an adequate model.
- (18) Failure to differentiate "the tree from the woods". This can lead to focusing the attention on specific aspects and ignoring other important ones.
- (19) Failure to document the model properly so that the assumptions and limitations are obscured.

3. Final Advice

The best advice for intended mathematical model builders is summed up in the following analogy due to Golomb [2].

A rocky road filled with pot-holes and a large sign in the foreground warning – PROCEED WITH CAUTION.

With this word of caution we come to the end of Part I.

Notes and References

The main reason for producing inadequate models is the failure to recognize the limitations of mathematical models. For further discussion on model uses and limitations, see [1]–[3].

Items [4]–[6] discuss pitfalls in modelling; [7] deals with pitfalls in data analysis; and [8] and [9] deal with pitfalls in computation.

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PART II

CASE STUDIES

CHAPTER 14

Dynamics of Malaria Spread

1 Introduction

Malaria is a tropical infectious disease which menaces more people in the world than any other disease. The World Health Organization reported in 1978 that, in Africa alone, one million children die annually from malaria before they reach the age of 5. It is conservatively estimated that malaria victims number around 100–200 million annually. Various schemes have been advocated for control of malaria but success has been limited. For the control strategies to be more efficient, improved epidemiological knowledge is required, including a better understanding of the population dynamics leading to the spread of malaria. In this context mathematical models play two important roles. Firstly, they help in clarifying the interaction between different variables of importance and lead to practical insights into the mechanisms underlying the observed phenomena. Secondly, they are useful in making a quantitative evaluation of the impact of different control strategies, so helping in the selection of optimal strategies for controlling the disease. In this chapter we focus our attention on building models to understand the process – in other words, to develop a mathematical theory for the spread of malaria. We commence with a brief discussion of the biology of malaria in Section 2. Section 3 studies the system characterization aspect. Section 4 looks at mathematical modelling in a general context and discusses the problems associated with data for parameter estimation and model validation. The remainder of the chapter deals with a variety of mathematical models. Each section discusses a specific model starting with the building and finishing with critical evaluation. We end with a concluding section which discusses further models that can be built.

2 Biology of Malaria

Malaria is an infectious parasitic disease in the sense that the disease is transmitted at some stage in the life cycle of a relevant organism (also called parasite) from an infected host to an uninfected host (also called susceptible).

The transmission of malaria is relatively easy to describe. The parasites causing malaria in humans are from the species of protozoa in the genus *Plasmodium*, and they are transmitted to humans by female mosquitoes belonging to certain species of the genus *Anopheles*. The female mosquitoes pick up the infection when they bite infected humans. Thus, the parasite has two hosts – humans and mosquitoes.

The *Plasmodium* life cycle can be described as follows. The parasite evolves through different stages during its life cycle. We start with the *sporozoite* stage – the stage where they reside in the salivary glands of infected female mosquitoes. When an uninfected human subject is bitten by an infected female mosquito, *Plasmodium* cells in the sporozoite stage are injected into the human blood. They are carried to the liver where they complete their growth and multiply asexually to produce *merozoites*. These then pass out of the liver into the blood stream and enter the red blood cells where further asexual reproduction takes place. In the process the red blood cells are destroyed, thus releasing more merozoites to attack healthy red blood cells. This cycle is repeated until the concentration of parasites in the blood reaches a high level, at which time the symptoms of malaria may appear in the host. The symptoms are chill, shivering, various aches and pains, etc. The *incubation period* is the time interval between the first bite and the appearance of clinical symptoms.

After a certain time the asexual reproduction of some merozoites comes to an end and distinct male and female *gametocytes* are formed in the red blood cells. When an uninfected female mosquito bites an infected human with *gametocytes* in the red blood cells, the gametocytes enter the new host. Once in the mosquito's stomach the *gametocytes* give rise to male and female *gametes*. The fertilization of the female *gametes* produce *zygotes* which go through a process of development resulting in a large number of sporozoites which migrate to the salivary gland. At this stage the infected female mosquito is capable of starting the *Plasmodium* life cycle all over again.

Thus, the parasite responsible for malaria in humans spends a part of its cycle in the human body and the rest in the mosquito. Humans are only an intermediate host harbouring the asexual phase of development while the mosquito is the final host as fertilization of eggs needed for sexual reproduction takes place there. It is interesting to note that the mosquitoes do not appear to be affected by the parasite in the manner in which humans are.

There are variations of detail between different species of *Plasmodium*, but the above description is adequate for our purpose – namely, building mathematical models to describe the population dynamics of malaria spread.

3 System Characterization

In Chapter 3 we defined system characterization as a simplified and idealized description of the real world relevant to the problem of interest, and in Chapter 4 we saw the role of it in the model building process. Since our

problem in this chapter is to understand the population dynamics of malaria, the system characterization involves describing variables relevant to the spread of malaria and the relationship between the variables. We have briefly discussed the role of *Plasmodium* as the parasite, and humans and mosquitoes as hosts in the spread of disease, in the previous section. In this section we examine other variables of interest and the framework for characterization.

3.1 Variables and Interactions

The variables of relevance are not too many. The variables can be described in different degrees of detail. We start with the simplest characterization and move on to a more detailed one.

(i) HUMAN POPULATION

In the simplest description one would divide the population into two groups – infected and uninfected. The uninfected are the group containing the susceptibles. One can characterize each group in terms of actual numbers, or as percentages of the total population. A slightly more detailed description is to divide the population into three groups – infected, susceptible and immune. We shall discuss immunity later on. A fairly detailed characterization is as follows. The total population is first divided into two categories – immune and non-immune. The non-immune category is divided into four groups – negative, incubating, positive infective and positive non-infective; the immune category is divided into three groups – negative, incubating and non-infective. In the above description an individual is called positive only if the parasite is in the blood, incubating if the parasite is in the liver, and negative if there are no parasites in the body. Individuals move from one group to another as they

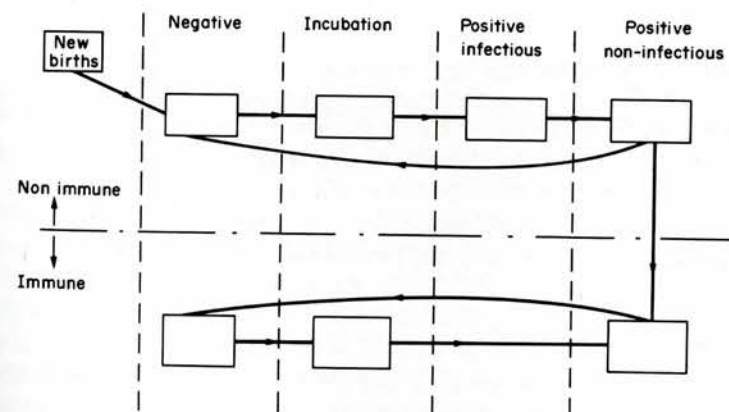


FIGURE 14.1 Grouping of human population into seven groups.

become infected or recover from an attack. A flow diagram for the last description is as shown in Figure 14.1. Note that the characterization ignores reduction in number due to deaths (either due to malaria or from other causes) but includes new births as they join the negative non-immune group.

The description becomes more detailed if we include factors such as age, quality of life, health standards, etc. The last two factors affect the transition from one group to another described above. The influence of age can be accounted for either by dividing the population into different age groups or by characterizing the population (total number or percentage) as a continuous function of age.

(ii) MOSQUITO POPULATION

As with the human population, the simplest description would divide the total population into two groups – infected and uninfected. A more refined description is to divide the infected group into two subgroups – infective and incubating. Where there is more than one species of malaria-carrying mosquito, we can either treat each species separately or ignore the variations between species.

(iii) PARASITE

We briefly discussed a simple characterization of the life cycle of *Plasmodium* in the previous section. Malaria in humans is caused by four different species belonging to the genus *Plasmodium*. The species are: *P. falciparum*, *P. malariae*, *P. vivax* and *P. ovale*. In the simplest characterization one would ignore the difference between the species, whereas a more detailed characterization would differentiate between them.

(iv) CLIMATIC AND GEOGRAPHICAL FACTORS

Climatic and geographical factors play an important role in the life cycle of mosquitoes. Pools of water are essential for mosquito breeding. Where this element is missing (e.g. deserts) the incidence of malaria is very low. Temperature is also an important factor. The sexual cycle of the parasite (characterized by the incubation period taking place in the mosquito from the acquisition of gametocytes to the production of sporozoites) depends both on the species of *Plasmodium* as well as on the temperature. As a consequence, malaria is confined to regions between 60°N and 40°S latitudes, and to places with altitude less than 3000 metres. Various parameters of relevance to the spread of malaria vary from region to region and must be estimated for each region.

(v) MOSQUITO/HUMAN INTERACTION

As indicated in the previous section, the onset of malaria in humans occurs at a certain stage in the life cycle of *Plasmodium*, and the life cycle requires interaction between mosquito and humans (in the form of the mosquito biting the human) with at least one of them being infected. The interaction can take place only when there is adequate contact. Adequate contact occurs by chance and hence must be characterized probabilistically. A parameter of high significance and interest is the probability of an adequate contact. If this is large (i.e. adequate contact occurs with high certainty) then the disease will spread to all susceptibles very quickly and we have an epidemic. If the probability is small, then the spread is relatively slow. The parameter characterizing the probability of an adequate contact depends on many factors – resistance of susceptible to infection; infectiveness of the infection; virulence of the parasite; quantity of parasite transmitted, etc.

In the simplest characterization we consider only the first adequate contact which infects the human, and treat the parasite in the human host as belonging to a single brood. In real life, multiple adequate contacts often occur over time, resulting in more than one brood of parasites being present in the one human host. This is called *superinfection*. A more detailed characterization would take this into account. In this case the infected human population must be divided into different groups based on the number of broods in the blood stream of individuals.

(vi) IMMUNITY

Immunity is of special importance as it acts as a barrier to uninfected humans getting infected when bitten by an infected mosquito. Immunity can arise in many ways – e.g. built up over time due to previous exposures; stimulated artificially by vaccination or immunization; genetic factors and so on. Accounting for immunity is difficult because of this wide range of possible sources.

3.2 Deterministic vs Stochastic Characterization

The spread of malaria requires the transfer of parasites from infected hosts to uninfected susceptible hosts. From the discussion so far, the two factors which are important are: (i) adequate contact resulting in bites which transfer parasites, and (ii) conditions to allow the life cycle of the parasite and mosquito to operate. The latter is influenced by changes in the season and can be treated as being deterministic. In contrast, the former is highly variable and, as discussed in Section 3.1, needs to be characterized probabilistically. As a result, when the human population is characterized by different groupings (as discussed in Section 3.1(i)) the transition between certain groups must be treated in a stochastic manner. However, if the human population is large

then, as an approximation, we can view the transition as being more or less deterministic and the rates of transmission between different groups given by the average values of the stochastic case. This approximation implies that the process can be modelled in a deterministic framework using mathematical formulations discussed in Chapter 5.

3.3 Time Scales

One can identify various time scales with regard to the biology and epidemiology of malaria. A few of the more important ones are listed below:

- (i) Time for sporozoite to enter the liver after being deposited into human blood by mosquito bite ~ 30 minutes.
- (ii) Incubation period – time between receiving the infection and the appearance of clinical symptoms ~ 10 – 30 days depending on the *Plasmodium* species.
- (iii) Cycles of attack (cyclical pattern of symptom occurrence, with symptoms being chill, shivering etc.) ~ 1 – 3 days depending on the type of malaria.
- (iv) Extrinsic incubation period (see Section 3.2(iv)) depends on the species of parasite as well as the external temperature. For the species *P. falciparum* we have the following figures.
 ~ 10 – 11 days when external temperature is 25°C ,
 ~ 15 – 17 days when external temperature is 23°C ,
 ~ 22 days when external temperature is 20°C .

Below 19°C the development of parasite is indefinitely retarded while above 32°C the proportion of parasites surviving drops off rapidly.

- (v) Life cycle of mosquito ~ 14 days.
- (vi) Life cycle of human ~ 70 – 80 years.
- (vii) Duration of immunity $\sim \geq 0$.

Let T be the time interval of study – i.e. we are interested in the population dynamics of malaria spread over this period. For the study to be meaningful, T should be ~ 1 – 10 years. If the changes to the human population are small over the time interval of study, we can ignore the variations and treat the total population as being constant. The number of mosquitoes can vary from season to season, but over a season we can approximate it as being roughly constant. Such assumptions simplify the system characterization and hence allow the use of simpler mathematical formulations (as dummies) in the modelling process.

3.4 Discrete vs Continuous Time Characterization

We can treat the time variable as being either continuous or discrete when building mathematical models to help our understanding of the spread of

malaria. If time is treated discretely, the interval of discretization most appropriate depends on the degree of detail incorporated into the model. Thus, if the incubation periods are being modelled explicitly, then an interval of discretization corresponding to a day is adequate. On the other hand, if the variables of the model are only numbers belonging to different groups, then larger intervals (e.g. week, month) would be appropriate. For the models to be presented in the next section, we will model time as a continuous variable.

4 Mathematical Modelling

A variety of models have been built to model the spread of malaria through the population. The earliest model is due to Ross, and was proposed in 1916. It is impossible to discuss all the models that have appeared since then. Here we shall discuss a series of six different models chosen to highlight the iterative nature of modelling where each subsequent model is an improvement over the earlier. The modelling of the spread of malaria is difficult, for the following reasons.

- (i) The mechanism for the spread of malaria is very complicated; hence great care needs to be taken to ensure a proper trade-off between the reality and the complexity of the model.
- (ii) The model parameters depend on geophysical location. Hence a model with a specified parameter set value for a particular region might not be valid for another region.
- (iii) The data available for parameter estimation, as well as for validation, are often limited and inadequate. In some instances the parameters can only be estimated based on a small section of the population – e.g. a cohort of newborn babies. In other instances, parameters must be obtained by specific field or laboratory experiments. We shall discuss some of these aspects when we consider specific model formulations.
- (iv) The problem of validation is difficult and requires combining forecasting abilities of the model with biological and epidemiological considerations.

Sections 5–9 deal with five deterministic model formulations which can be viewed as a progressive sequence of improved models. In Section 10 we examine a stochastic model.

5 Model I (Ross, 1916)

This model was first formulated by Ross in 1916 [5]. The spread of malaria is characterized as a deterministic process and the approach taken is the “black-box” approach as the system is characterized through a single variable representing the proportion of the human population affected by malaria.

5.1 Model Formulation

Let $x(t)$ represent the proportion of human population affected by malaria at time t . As a result, the proportion unaffected is $1 - x(t)$. Changes to $x(t)$ over time occur due to unaffected people getting infected, and affected people recovering. Note that the model does not differentiate between infectious and non-infectious in the group of affected people, nor between susceptibles and immunes in the unaffected group. Let r represent the recovery rate (i.e. proportion of affected people who recover in a unit time) and h represent the proportion of unaffected people receiving infectious bites per unit time. It is assumed that these two parameters do not change with time.

Thus, changes to $x(t)$ in a small interval Δt are given by

$$x(t + \Delta t) - x(t) = \{h(1 - x(t)) - rx(t)\}\Delta t \quad (1)$$

which in the limit $\Delta t \rightarrow 0$ yields

$$dx(t)/dt = h - (r + h)x(t) \quad (2)$$

i.e. the model involves a simple linear first-order ordinary differential equation formulation.

If the proportion of infected at time $t = 0$ be given by

$$x(0) = x_0 \quad (3)$$

then the model is completely specified by (2) and (3).

The parameter set is given by

$$\theta = \{r, h\} \quad (4)$$

with the constraint

$$\Theta = \{r \geq 0; h \geq 0\}.$$

5.2 Model Analysis

It is easily seen that $x(t), t \geq 0$ is given by

$$x(t) = \{h/(r + h)\} - \{[h/(r + h)] - x_0\}e^{-(r+h)t} \quad (5)$$

As $t \rightarrow \infty$, we have the asymptotic value $x(\infty)$, which is given by

$$x(\infty) = h/(r + h) \quad (6)$$

and this corresponds to the proportion of infected population under what is called the endemic condition.

Some special cases are as follows:

- (i) $r = 0, h > 0 \rightarrow x(\infty) = 1$; i.e. the whole population is infected.
- (ii) $r > 0, h = 0 \rightarrow x(\infty) = 0$; i.e. the infection disappears
- (iii) $r = 0, h = 0 \rightarrow x(\infty) = x_0$; i.e. there is no change.

If we concentrate on newborn children, then $x_0 = 0$, which yields

$$x(t) = \{h/(h + r)\} \{1 - e^{-(r+h)t}\} \quad (7)$$

(Note: In the above case, $x(t)$ represents the proportion of newborn population affected by malaria at time t .) Let $p(t)$ represent the population of infected people detected at time t using some testing procedure. If the testing procedure is perfect, then $p(t) = x(t)$. However, if an infected person is detected with probability k ($0 < k \leq 1$) then we have

$$p(t) = kx(t) = \{kh/(h + r)\} \{1 - e^{-(r+h)t}\} \quad (8)$$

The above equation will play an important role in parameter estimation, with k being treated as an additional parameter.

5.3 Parameter Estimation

By observing the spread of malaria in a cohort of newborn children, we can use (8) to obtain estimates for the parameters of the model. Let n_i represent the number of children observed, and a_i the number found to be infected at time t_i , $1 \leq i \leq I$. Then the estimates can be obtained by minimizing

$$\sum_{i=1}^I \{p(t_i) - (a_i/n_i)\}^2 \quad (9)$$

where $p(t_i)$ is given by (8).

An alternative statistical approach is to view a_i as being the number of children infected in a population n_i at t_i when the probability of being infected is given by p_i . As a result, the likelihood of observing a_i , $1 \leq i \leq I$ given n_i , $1 \leq i \leq I$, is given by

$$\sum_{i=1}^I K_i (p_i)^{a_i} (1 - p_i)^{(n_i - a_i)} \quad (10)$$

where K_i is given by

$$K_i = \{a_i! (n_i - a_i)! / n_i!\}$$

and is independent of the parameters to be estimated. Note that the unknown parameters enter through $p_i = p(t_i)$, with $p(t_i)$ given by (8). The log-likelihood function is given by

$$L = \hat{K} + \sum_{i=1}^I \{a_i \log p_i + (n_i - a_i) \log(1 - p_i)\} \quad (11)$$

where $\hat{K}$ is a constant independent of the parameters to be estimated. The estimates are obtained by maximizing L with respect to the parameters.

Bailey (1982) [3] obtained parameter estimates using data from Pull and Grab (1974) [11] but aggregated monthly. The aggregated data is given in Table 14.1, and the value of t_i used for each interval is the central point of the

TABLE 14.1 Aggregated Monthly Data for Observed Proportion of Infected [3]

Age interval i	Central point t_i	Number inspected n_i	Number found positive a_i	Observed proportion of infected $p_i = a_i/n_i$
1	45	202	26	0.129
2	75	235	76	32.3
3	105	210	91	43.3
4	135	210	93	44.3
5	165	243	140	57.6
6	195	219	121	55.3
7	225	219	128	58.4
8	255	241	135	56.0
9	285	179	121	60.8
10	315	204	118	57.8
11	345	205	132	64.4

interval. Note that for the data used $I = 11$. The estimates obtained by Bailey are as shown below. Figure 14.2 shows the fit between the model output and the observed data indicating a reasonably good fit.

$$\left. \begin{aligned} \hat{h} &= 0.0089 \pm 0.00059 \\ \hat{r} &= 0.00050 \pm 0.00148 \\ \hat{k} &= 0.637 \pm 0.078 \end{aligned} \right\} \quad (12)$$

Since r is very small, we can treat it as being zero for young children and regard h and k as the two unknown parameters. The estimates obtained by Bailey (1982) [3] are given by

$$\left. \begin{aligned} \hat{h} &= 0.0081 \pm 0.00054 \\ \hat{k} &= 0.662 \pm 0.024 \end{aligned} \right\} \quad (13)$$

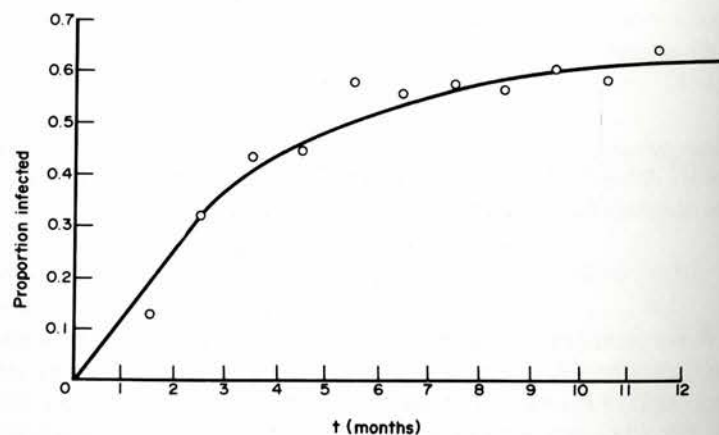


FIGURE 14.2 Comparison of Model I response and observed data (○).

5.4 Validation

One way of validating the model is through the goodness-of-fit between model prediction and the observed data. This would require a statistical test and Bailey [3, p. 150] uses the χ^2 test to validate the above model.

Another way to evaluate the model is in terms of its qualitative behaviour. In the above model, as well as in the many cases studied by Macdonald ([4], [6]) using a cohort of newborn babies, the value for r obtained is very low. Since the reciprocal of r corresponds to the duration for which a person stays infected, once bitten by an infectious mosquito, $r = 0.0005$ corresponds to an infection lasting 6 years. This is in strong disagreement with the actual average period of infection. Hence the validity of the model with r very small is doubtful.

It is worth noting that the small values obtained for r involved field data for newborn babies; hence one might infer that r is small only in the early stages of life, and that it increases with age. If this be the case, then the above model must be rejected, as it assumes the recovery rate to be a constant independent of age.

Finally, the model is a gross over-simplification of the process for the spread of malaria, for it ignores many features – e.g. mosquito population, incubation period, uncertainty in the spread, to name a few.

6 Model II (McDonald, 1950)

This model was first proposed by Macdonald [6] with the mathematical development done in conjunction with Irwin; hence it is sometimes called the “Macdonald–Irwin model”. This model was built to overcome the deficiency of Model I, which yielded very low values for r when fitted to real data. The model is built using the concept of superinfection, which assumes that the human host can carry multiple broods of parasite and is in infected state as long as there is at least one brood present. Unfortunately, the precise notion of multiple broods is not explicit in the model formulation.

6.1 Model Formulation

We use the notation of the earlier model. The model is given by

$$\left. \begin{aligned} dx(t)/dt &= h - rx(t) & h \leq r \\ &= h(1 - x(t)) & h \geq r \end{aligned} \right\} \quad (14)$$

An intuitive justification is as follows. If $h < r$, then in time Δt all individuals, whether infected or not, exhibit new infection at a rate $h\Delta t$. Thus, the change in $x(t)$ over Δt is given by

$$\{h - rx(t)\}\Delta t \quad (15)$$

If $h > r$, then once infected the individual would never recover; hence change in $x(t)$ over Δt is given by

$$h(1 - x(t)) \quad (16)$$

In the limit $\Delta t \rightarrow 0$, we have (14) as a consequence of (15) and (16). The model is completely specified by specifying the proportion of population infected at time $t = 0$, i.e. by x_0 given by (3).

6.2 Model Analysis

It is easily seen that $x(t)$ satisfying (14) is given by

$$x(t) = \begin{cases} (h/r)\{1 - e^{-rt}\}, & h \leq r \\ 1 - e^{-ht} & h \geq r \end{cases} \quad (17)$$

As $t \rightarrow \infty$ the asymptotic value is given by

$$x(\infty) = \begin{cases} (h/r), & h \leq r \\ 1, & h \geq r \end{cases} \quad (18)$$

For a small value of r , $x(t)$ obtained from this model is very close to that obtained from Model I (equation (7)).

6.3 Parameter Estimation

Using various bodies of field data, Macdonald [6] obtained estimates for r closer to the realistic values of $r \sim 0.005$. Thus the model is an improvement over Model I from this point of view.

6.4 Validation

As mentioned earlier, the model is an improvement in the sense that it yields more realistic values for the parameter r . Unfortunately the model does not truly incorporate the original concept of multiple broods of parasite in the body as formulated by Macdonald. In addition, the model suffers from the over-simplification discussed in Model I.

7 Model III (Dietz, 1970)

This model was first developed by Dietz [7] to represent adequately the concept of superinfection formulated by Macdonald, and is called the "Macdonald-Dietz model". The characterization is done through the total population being divided into different groups based on the number of broods present in an individual. Thus, individuals belonging to group j carry j broods of parasite in their bodies. If $j = 0$ then the group is the collection of individuals unaffected by malaria. As in the earlier models, the characterization of the mechanism for the spread is done in a deterministic framework.

7.1 Model Formulation

Let $f_j(t)$, $0 \leq j < \infty$, represent the proportion of the total population with exactly j broods. If $x(t)$ is the proportion affected by malaria at t , we have

$$x(t) = \sum_{j=1}^{\infty} f_j(t) \quad (19)$$

and the unaffected proportion given by

$$1 - x(t) = f_0(t) = 1 - \sum_{j=1}^{\infty} f_j(t) \quad (20)$$

In an interval Δt , a change in $f_j(t)$ can occur when one or more persons in group $(j-1)$ is bitten by an infectious mosquito resulting in an increase in the number of broods by one in the bitten individual, or when one or more persons in group $(j+1)$ recovers partially so that the number of broods in the infected person is reduced by one.

Let r define the recovery rate for individual brood and h be the rate of new infections being introduced. We have the increase in $f_j(t)$ in time Δt given by

$$\{hf_{j-1}(t) + r(j+1)f_{j+1}(t)\}\Delta t \quad (21)$$

and the decrease in $f_j(t)$ given by

$$\{(h+rj)f_j(t)\} \quad (22)$$

Using a limiting argument we have the model given by the following set of equations:

$$\left. \begin{aligned} df_0(t)/dt &= -hf_0(t) + rf_1(t) \\ df_j(t)/dt &= hf_{j-1}(t) - (h+rj)f_j(t) + r(j+1)f_{j+1}(t), \quad j \geq 1 \end{aligned} \right\} \quad (23)$$

The model is completely specified once the distribution at $t = 0$ is specified; i.e.

$$\left. \begin{aligned} f_j(0) &= f_j^0 \quad (0 \leq j \leq \infty) \\ (\text{with } f_j^0 &\geq 0 \text{ and } \sum_{j=0}^{\infty} f_j^0 = 1) \end{aligned} \right\} \quad (24)$$

is given; $x(t)$, the proportion infected, is given by (19).

7.2 Model Analysis

We shall obtain the solution for the case applicable for a cohort of newborn babies. In this case, (24) is given by

$$f_0^0 = 1; \quad f_j^0 = 0, \quad 1 \leq j \leq \infty \quad (25)$$

Define

$$F = F(\omega, t) = \sum_{j=0}^{\infty} \omega^j f_j(t) \quad (26)$$

Then multiplying (23) by ω^j and summing over all j we have

$$\partial F / \partial t = h(\omega - 1)F - r(\omega - 1)\partial F / \partial \omega \quad (27)$$

and from (24) and (25) we have

$$F(\omega, 0) = 1 \quad (28)$$

Equation (27) is a first-order linear partial differential equation and can be solved to yield

$$F(\omega, t) = \exp \{ - (h/r)(\omega - 1)(1 - e^{-rt}) \} \quad (29)$$

From (19) we have

$$\begin{aligned} x(t) &= 1 - f_0(t) = 1 - F(0, t) \\ &= 1 - \exp \{ - (h/r)(1 - e^{-rt}) \}. \end{aligned} \quad (30)$$

As $t \rightarrow \infty$ we have the asymptotic result

$$x(\infty) = 1 - \exp(-h/r) \quad (31)$$

which yields the proportion affected under endemic conditions.

Let $p(t)$ represent the proportion of infected people detected at time t using some testing procedure. If the procedure is perfect, then $p(t) = x(t)$. If the testing procedure is not perfect, then the proportion of observed infected people at time is given by $p(t) = kx(t)$, with $0 < k \leq 1$.

7.3 Parameter Estimation

The procedure for estimating the parameters (viz. h , r and k) is essentially similar to that discussed in Section 5.3. Using the cohort of newborn babies with a_i , n_i and t_i as defined in Section 5.3 we have the log-likelihood function given by (12) with p_i given by

$$p_i = k[1 - \exp \{ - (h/r)[1 - \exp(-rt_i)] \}] \quad (32)$$

For the data given in Table 14.1, the estimates for the parameters are nearly the same as that given in (12). This follows, as for small values of r , p_i obtained from (32) is nearly the same as that obtained from (8).

7.4 Validation

The comments of Section 5.4 are equally applicable here, so we shall not repeat them. However, the model is an improvement as it incorporates the concept of superinfection.

8 Some Comments

In the previous three sections we discussed three deterministic models for the spread of malaria. In this section we comment on the models studied so far, so

as to give a better insight and provide a basis for some new model formulations.

- (i) The models are over-simplified.
- (ii) The models discussed so far do not characterize the mosquito population and the interaction between humans and mosquitoes.
- (iii) The models are deterministic, whereas the interaction and spread are highly stochastic.
- (iv) The parameters r and h were obtained using data for observed proportions of infected in the cohort of newborn babies. These parameters need to be related to more basic parameters of the process for the spread of malaria.

In this section we discuss (iv). Improved models which overcome the limitations discussed in (i)–(iii) are studied in subsequent sections.

In addition to x , r and h , defined earlier, we employ the following symbols. Our presentation follows along the lines of Bailey [3].

- m : mosquito density per human
- a : average number of humans bitten per day per mosquito
- s : proportion of mosquitoes with sporozoites in their salivary gland
- b : proportion of mosquitoes, having sporozoites in their salivary glands, that are actually infectious
- n : extrinsic incubation period
- p : probability that a given mosquito survives over a given day
- γ : mosquito death rate.

From general biological consideration we have

$$h = masb \quad (33)$$

We assume that, once infected, the mosquito stays infected for the remainder of its life. A mosquito gets infected only when an adequate contact is made with an infected person. Because of the extrinsic incubation period there are no infected mosquitoes with age $< n$. Thus, if we assume that adequate contacts between a mosquito of age $t > n$ and infected humans is given by a Poisson process with parameter $xa(t - n)$, then the probability of at least one adequate contact is given by

$$1 - \exp(-xa(t - n)) \quad (34)$$

Thus the proportion of infected mosquitoes of age t to $t + dt$ is given by

$$\{1 - \exp(-xa(t - n))\} \gamma e^{-\gamma t} dt \quad (35)$$

and by integrating (35) from n to ∞ we obtain the overall proportion of infected mosquitoes which corresponds to s . In other words, we have

$$s = axe^{-\gamma n}/(ax + \gamma) \quad (36)$$

Since the mosquito death rate is γ , the probability that a mosquito survives one day is given by

$$p = e^{-\gamma} \quad (37)$$

Substituting (37) in (36) we obtain

$$s = axp^n/(ax - \log p) \quad (38)$$

and from (33) we have

$$h = (ma^2bxp^n)/(ax - \log p) \quad (39)$$

This shows explicitly the dependence of h on the various basic parameters of the mechanism and the human/mosquito interaction. Some of the basic parameters can be obtained by field observations or controlled laboratory experimentation. The basic parameters change with geographical location as well as seasonally.

Some estimates for the parameter values are given in Bailey [3, Ch. 9] and references cited therein.

9 Model IV (Dietz, Molineaux and Thomas, 1974)

This model was developed in close co-operation with epidemiologists, entomologists and immunologists in connection with a field project in the district of Garki in Northern Nigeria [8]. The spread is modelled as a deterministic process but the system characterization is more detailed. The total population is divided into seven different groups, as shown in Fig. 14.1 and briefly discussed in Section 3.1(i). The rate of transfer between groups is related to some basic parameters, and as such the model incorporates a high degree of realism.

9.1 Model Formulation

We use the symbols defined in the original paper. The variables refer to the proportion of the human population in the seven different groups as a function of time. The variables defining the different groups are as follows.

- $x_1(t)$: non-immune/negative
- $x_2(t)$: non-immune/incubating
- $y_1(t)$: non-immune/positive infections
- $y_2(t)$: non-immune/positive – non-infectious
- $x_3(t)$: immune/negative
- $x_4(t)$: immune/incubating
- $y_3(t)$: immune/positive – non-infectious

The rates for transition between different groups are given as follows.

- $h(t)$: from “negative” to “incubating” for both non-immune and immune;
- $Q(t)$: from incubating to infectious in the case of non-immune and from incubating to non-infectious in the case of non-immune;
- α_1 : from infectious to non-infectious in the non-immune;
- α_2 : from non-immune non-infectious to immune non-infectious;
- R_1 : from non-infectious positive to negative in non-immune;
- R_2 : from non-infectious positive to negative in immune category.

In addition, we define

- n : fixed incubation period;
- η : extrinsic incubation period;
- δ : rate of new births as well as death rate for all groups.

Using a discrete time characterization with the discretization time interval being unity, we have, from simple balancing, the changes to the various proportions given by the following set of equations:

$$\left. \begin{aligned} \Delta x_1 &= \delta + R_1 y_2 - (h + \delta)x_1 \\ \Delta x_2 &= hx_1 - Qx_1(t-n) - \delta x_2 \\ \Delta x_3 &= R_2 y_3 - (h + \delta)x_3 \\ \Delta x_4 &= hx_3 - Qx_3(t-n) - \delta x_4 \\ \Delta y_1 &= Qz_1(t-n) - (\alpha_1 - \delta)y_1 \\ \Delta y_2 &= \alpha_1 y_1 - (\alpha_2 + R_1 + \delta)y_2 \\ \Delta y_3 &= \alpha_2 y_2 - Qx_3(t-n) - (R_2 + \delta)y_3 \end{aligned} \right\} \quad (40)$$

(Note: We have suppressed the argument t for most of the variables. Because of the incubation period there is a time lag of n . Hence some of the variables are the lagged variables (i.e. at time $t-n$) and these are shown explicitly.)

We omit the details of the derivation which relate some of the rate functions to more basic parameters. The final form is given by

$$\left. \begin{aligned} Q &= (1 - \delta)h(t-n) \\ h &= g[1 - \exp\{-C(t-n)y_1(t-n)\}] \\ R_i &= h/\{\exp(h/r_i) - 1\}, 1 \leq i \leq 2 \end{aligned} \right\} \quad (41)$$

where $C(t)$ is a function which is called “vectorial capacity” and characterizes the relevant information of mosquito population and r_i ($1 \leq i \leq 2$) representing rate of elimination for a given brood. Defining q_i to be probability of detecting the presence of parasite, then the proportion of population

detected to be positive is

$$p(t) = \sum_{i=1}^3 q_i y_i(t) \quad (42)$$

and the true proportion which is positive is given by

$$x(t) = \sum_{i=1}^3 y_i(t) \quad (43)$$

If one assumes that $q_1 = q_2$, then the model has 10 parameters given by

$$\theta = \{\delta, r_1, r_2, q_1 (=q_2), q_3, n, \alpha_1, \alpha_2, g, \gamma\} \quad (44)$$

(Note: We need to specify the vectorial capacity $C(t)$ using entomological considerations, and once this is done the model is completely specified by specifying the values for the seven variables at $t = 0$.)

9.2 Model Analysis

It is not possible to obtain an analytical solution to the set of difference equations given by (40). The form of the model makes it ideally suited for implementation on a digital computer; hence such solutions are easily obtained.

9.3 Parameter Estimation

Dietz *et al.* [8] fitted the model to two different populations with widely varying levels of vectorial capacity. They assumed values for seven parameters based on entomological and biological considerations, and the values assumed are as follows:

$$\left. \begin{aligned} \delta &= 0.0001 \\ r_2/r_1 &= 10 \\ q_1 (=q_2) &= 1 \\ q_3 &= 0.7 \\ \gamma &= 10 \text{ days} \\ n &= 15 \text{ days} \\ \alpha_1 &= 0.002 \end{aligned} \right\} \quad (45)$$

The remaining three parameters were estimated using field data and are as follows.

$$\begin{aligned} \hat{\alpha}_2 &= 0.00019 \pm 0.0001 \\ \hat{g} &= 0.097 \pm 0.017 \\ \hat{r}_1 &= 0.0023 \pm 0.0005 \end{aligned} \quad (46)$$

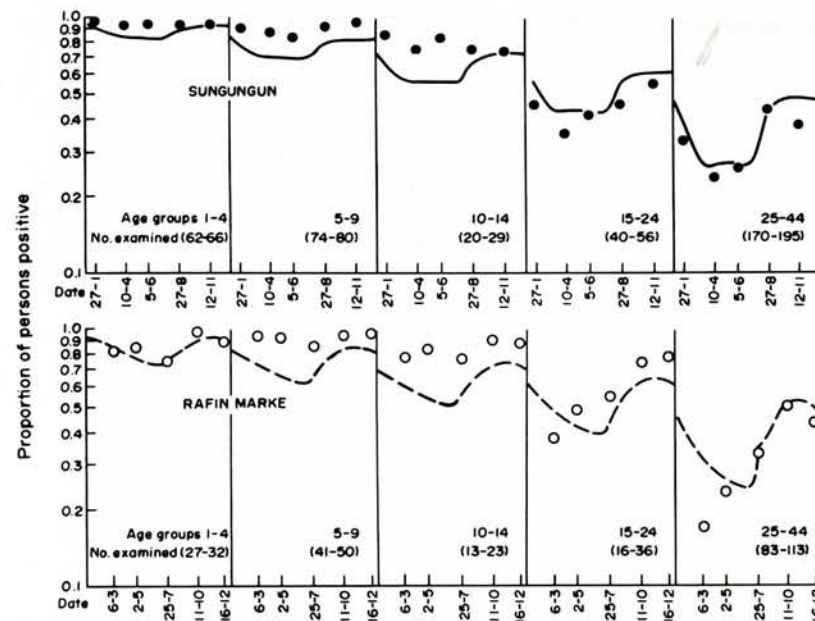


FIGURE 14.3 Comparison of observed (●, ○) and Model IV response (—, ---).

Figure 14.3 is a reproduction of a figure given in Dietz *et al.* [8] which shows the comparison between the model output obtained using the above set of parameters and some observed field data.

9.4 Validation

With the restricted data available for estimation it is generally agreed by experts that the model is an adequate representation for the spread of malaria. However, the assumption that the mechanism for the spread is deterministic is not justifiable. Hence a stochastic model which overcomes this drawback would yield an even better model. We discuss one such.

10 Model V (Bekessy, Molineaux and Storey, 1976)

The models discussed so far (Models I-IV) are deterministic – i.e. the changes to $x(t)$, the proportion of total population infected, are given by a deterministic formulation. In this section we discuss a model which characterizes the change from infected to uninfected or vice-versa by an uncertain chance mechanism.

10.1 Model Formulation

Define N and $X(t)$ as follows:

N : total population (assumed fixed),

$X(t)$: number of individuals infected at time t .

As a result we have

$N - X(t)$: number of susceptibles at time t .

We assume that the probability of one new infection occurring in time t to $t + \Delta t$ is given by $h(N - X(t))\Delta t$ and the probability of one recovery in the same time period by $rX(t)\Delta t$.

10.2 Model Analysis

Define $p_j(t)$ and $P(z, t)$ as follows:

$$p_j = \text{prob}\{X(t) = j\} \quad 0 \leq j \leq N \quad (47)$$

and

$$P(z, t) = \sum_{j=0}^N p_j(t) z^j \quad (48)$$

Then, using a method similar to that used in Section 7.1 for obtaining $f_j(t)$, we have p_j satisfy the following set of differential equations:

$$\begin{aligned} dp_0(t)/dt &= -hNp_0(t) + rp_1(t) \\ dp_j(t)/dt &= -\{h(N-j) - rj\}p_j(t) + h\{N-j+1\}p_{j-1}(t) \\ &\quad + r(j+1)p_{j+1}(t) \end{aligned} \quad (49)$$

for $1 \leq j \leq N-1$, and

$$dp_N(t)/dt = -rNP_N(t) + hp_{N-1}(t)$$

and $P(z, t)$ satisfies the partial differential equation

$$\partial P / \partial t = (1-z)(r+hz)\partial P / \partial z + \gamma h(z-1)P \quad (50)$$

If we assume that, at $t = 0$, the number of infected individuals is given by

$$x(0) = a \quad (51)$$

then

$$p_j(0) = \begin{cases} 1 & \text{if } j = a \\ 0 & \text{otherwise} \end{cases} \quad (52)$$

and

$$P(z, 0) = z^a$$

With the above initial condition, (50) can be solved analytically to yield

$$\begin{aligned} P(z, t) &= (r+h)^{-N} \{(r+hz) + r(z-1)e^{-(r+h)t}\}^a \cdot \{(r+hr) \\ &\quad - h(z-1)e^{-(r+h)t}\}^{N-a} \end{aligned} \quad (53)$$

From this, we can obtain expressions for various moments of $X(t)$. Let

$$m(t) = E[X(t)]/N \quad (54)$$

represent the mean value for the fraction of people infected at time t . Then, from (53) we have

$$\begin{aligned} E[X(t)] &= [\partial P / \partial z]_{z=1} \\ &= \{Nh/(r+h)\} \{1 - e^{-(r+h)t}\} \end{aligned} \quad (55)$$

and substituting this in (54) yields

$$m(t) = \{h/(r+h)\} \{1 - e^{-(r+h)t}\} \quad (56)$$

This is identical to $x(t)$ in Model I. Thus, this model can be viewed as a stochastic version of Ross's model.

10.3 Parameter Estimation

In stochastic modelling, one can estimate the model parameters by various methods – e.g. method of moments; maximum-likelihood, etc. The derivation of the maximum-likelihood estimator follows along the lines indicated in Section 5.3 and is omitted.

10.4 Validation

One way of validating is to evaluate the goodness-of-fit between the estimated mean of $X(t)$ based on the data available and the mean of $X(t)$ obtained from the model. This can be done in a manner similar to that discussed in Section 5.4.

The main criticism of the model is that it treats individuals as being either infected or not. This is a gross over-simplification and hence the model is suspect. An extension to include different groups (as done in Model IV) would make the model more realistic.

11 Conclusions

In this chapter we have examined five different models for the population dynamics of malaria spread. The reason for the choice was to illustrate the iterative nature of modelling where one starts with the simplest model and improves it at each stage to produce a better one. Many other models have been developed and applied with varying degrees of success. Notes at the

end of the chapter give references to sources where more details of these can be found.

Notes and References

Most books on infectious diseases contain a chapter on malaria. See for example [1] and [2]. There is a large number of books dealing specifically with malaria (e.g. [3] and [4]). In particular, the book by Bailey deals with a variety of mathematical models that have been developed. We have examined only a few of these in this chapter. For further details of the models discussed in this chapter, see either [4] or [5]–[8]. For other models see Bailey [4] and the references cited therein. An excellent source for more information, including data about the spread of malaria, is [9]. There are many papers in the above journal which give field data from different parts of the world.

The modelling of different control actions and their effect on the spread of malaria is still at an infancy stage and mainly of theoretical interest. A review of models for the control of infectious diseases until 1977 can be found in [10]. Since then a few more models have been developed, some being for the control of the spread of malaria, but in general they are highly oversimplified and inadequate for practical implementation (e.g. [11]).

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CHAPTER 15

Designing a Pneumatic Pump

1 Introduction

In an aquarium it is essential that there be a good supply of dissolved oxygen to maintain the health of the fish and other life inside the tank. This is often achieved by pumping air into the aquarium. The performance of the pump depends on its design, which in turn involves two phases. The first is a conceptual design in which a suitable scheme is developed. This involves identifying the different components and the coupling between components necessary for a solution. The second phase deals with the specification of components in terms of their size, characteristics and other functional parameters so that the pump performance meets some stated criterion. In this chapter we shall concentrate on the second phase. More specifically, we are interested in predicting the performance of a small pneumatic pump, suitable for domestic aquariums, as a function of the characteristics of its components. We build a sequence of models, of increasing complexity, to achieve that.

In Section 2 we carry out the system characterization. We take a “white-box” approach for two reasons: firstly, the mechanics of pump operation are well understood and hence possible to describe explicitly; secondly, such an approach is essential to relate the performance of the system to the characteristics of individual components. The characterization, and model representations, are best done using bond-graphs. The bond-graph technique is a powerful generalized technique which is particularly useful in modelling dynamic systems that can be described in terms of energy flows and transformations. A brief introduction to bond-graphs is given in Section 3. In Section 4 the bond-graph technique is applied to building a sequence of models of the air pump. Throughout the sequence there is progressive refinement of the model with a critical analysis of the effect of each refinement. Since there are no performance data available (as the problem is a design problem and the pump is yet to be built) this critical evaluation can be viewed as “model validation”. In Section 5 we discuss the analysis of the final model to obtain the end-product – viz. relating pump performance to component characteristics. We conclude with some general comments about the modelling process in Section 6.

2 System Characterization

A schematic representation of the conceptual scheme for a simple pneumatic pump is shown in Figure 15.1. The pump can be viewed as a system. The boundary (or interface) between the system and its environment is shown in Figure 15.2. The system receives electric power and air (at atmospheric pressure) from the environment, and in turn supplies air (at a pressure higher than the atmospheric pressure) to the aquarium, which is a part of the environment. The components of the system are:

- (1) electromagnetic coil
- (2) magnet
- (3) lever
- (4) bellows
- (5) inlet and outlet valves
- (6) pipes (or tubes) for flow of air.

The pump operating mechanism is fairly simple. When an alternating voltage from the mains supply is applied across the coil, an alternating

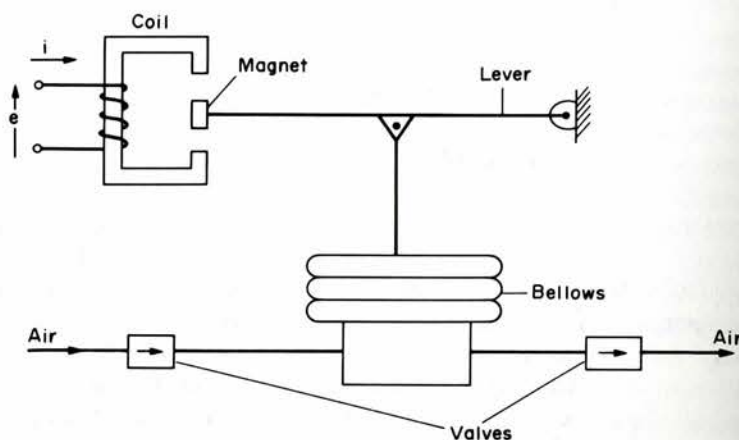


FIGURE 15.1 Schematic representation of a simple pneumatic pump.

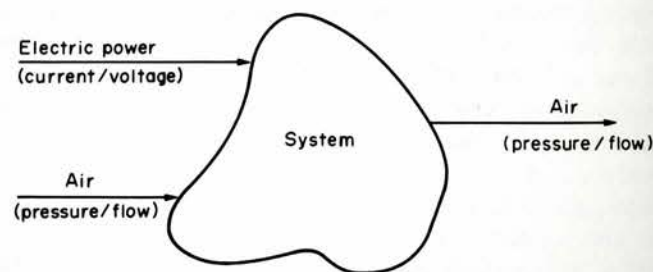


FIGURE 15.2 System/environment interface.

magnetic field is set up. This field interacts with the magnet to produce an oscillating motion (in a vertical plane) of the magnet. This motion is transmitted through the lever to produce a vertical motion of the bellows. When the bellows move up, air is drawn through the inlet valve (with outlet valve closed) and when it moves down, air is pumped through the outlet valve (with inlet valve closed).

A better understanding of the mechanism is achieved by viewing the system in terms of the energy transformation. From this point of view the system can be described as follows. Electrical energy is transformed into mechanical energy, which in turn is transformed into pneumatic energy. Since the device operates continuously, energy flow, or power, is more appropriate to describe the system. Thus, electrical power (given by the product of voltage and current) is transformed into mechanical power (given by the product of force and velocity) which in turn is transformed into pneumatic power (given by the product of pressure and flow rate).

The variables characterizing the components can be described using terms from different theories in physical sciences. The terms that will be used are: mass, damping coefficient, force, velocity from dynamics; resistor, inductance, voltage, current from electrical circuit theory; pressure and flow rate from fluid mechanics. The relationships between the variables are given in terms of the laws of these theories.

The components or devices (listed earlier) can be divided into three types:

- (i) energy (or power) transforming devices,
- (ii) energy storage devices, and
- (iii) energy dissipation devices.

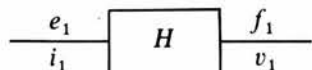
Viewed from an energy (or power) transformation point of view, the three main components of the system are: electromagnetic actuator, lever and bellows. In the simplest characterization these can be viewed as couplers. A coupler is a device which transforms energy (or power) with a power conserving relationship. Both the input and output are characterized through two variables: one called "effort variable" and the other called "flow variable". The product of the two input variables gives the power inflow and the product of the two output variables gives the power outflow. In a coupler the power output equals the power input, and the output flow and effort variables are related to the input flow and effort variables by a simple algebraic relationship.

The effort and flow variables associated with electrical, mechanical and pneumatic power are as follows:

	Effort variable		Flow variable	
Electrical	Voltage	(e)	Current	(i)
Mechanical	Force	(f)	Velocity	(v)
Pneumatic	Pressure	(p)	Flow rate	(q)

With this background we are in a position to characterize the three main components mentioned earlier.

The electromagnetic actuator is a coupler which transforms electrical power into mechanical power. It can be represented schematically as shown below:

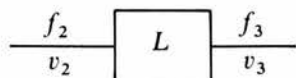


where e_1 represents the voltage across the coil; i_1 the current in the coil; f_1 the force acting on the magnet and v_1 the velocity with which the magnet is moving. The relationship between the output variables and the input variables are given by

$$\left. \begin{aligned} v_1 &= (1/H)e_1 \\ f_1 &= Hi_1 \end{aligned} \right\} \quad (1)$$

where H is a constant. Note that the two gains (i.e. H and $1/H$) are reciprocals of each other and the product $v_1 f_1 = e_1 i_1$, signifying power conservation.

The lever is a coupler in which both the input and the output power are mechanical. A schematic representation of this is as shown below:

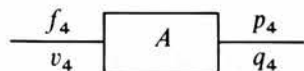


with the variables related by

$$\left. \begin{aligned} f_3 &= (1/L)f_2 \\ v_3 &= Lv_2 \end{aligned} \right\} \quad (2)$$

where L is the lever ratio. Note again that $f_3 v_3 = f_2 v_2$, signifying power conservation.

Finally the bellows, viewed as a coupler, can be represented by a schematic diagram as shown below:



with

$$\left. \begin{aligned} p_4 &= (1/A)f_4 \\ q_4 &= Av_4 \end{aligned} \right\} \quad (3)$$

where A is the cross-sectional area of the bellows, and again we have $f_4 v_4 = q_4 p_4$.

The other components are listed below in terms of their relative importance. Each is identified as either an energy storage device (ES) or energy dissipation device (ED):

- (i) mass of magnet (ES), compliance of rubber bellows (ES);
- (ii) resistance of coil (ED), inductance of coil (ES);

- (iii) internal damping in rubber bellows (ED);
- (iv) friction at lever pivot (ED);
- (v) air friction at inlet and outlet valve (ED);
- (vi) compressibility of air (ES).

Each component needs to be characterized by an appropriate flow and an effort variable and a relationship between the two. We shall do this in the next section, using the bond-graph approach.

3 Bond-Graphs: an Introduction

Table 15.1 contains the main symbols for bond-graphs that will be used later in the chapter. A simple bond is represented by a straight line with the effort

TABLE 15.1 Bond-graph Symbols

Variables, power, causality

$\frac{e}{f}$	simple bond; effort (e) on top and flow (f) on bottom
$\rightarrow$	half-arrow to indicate positive power flow
$- $	causal stroke: effort to right, flow to left
$ $	causal stroke: effort to left, flow to right
$\leftarrow$	positive power flow and effort to left

One-port elements

$-X$	$X = R, L, \text{ or } C$ (electrical) $= D, M, \text{ or } K$ (mechanical)
------	--

Two-port elements

$\frac{e_1}{f_1} \text{ TF } \frac{e_2}{f_2}$	Transformer	$e_2 = ke_1$ $f_1 = kf_2$
$\frac{e_1}{f_1} \text{ GY } \frac{e_2}{f_2}$	Gyrator	$f_2 = le_1$ $f_1 = le_2$

Three-port elements

$\frac{e_1}{f_1}$	1	$\frac{e_2}{f_2}$	1-Junction
	$f_3 e_3$		$e_1 + e_2 + e_3 = 0$ $f_1 = f_2 = f_3$
$\frac{e_1}{f_1}$	0	$\frac{e_2}{f_2}$	0-Junction
	$f_3 e_3$		$e_1 = e_2 = e_3$ $f_1 + f_2 + f_3 = 0$

variable on top and the flow variable below. A half-arrow indicates the direction of positive power flow and a cross-stroke indicates causality.

One-port elements are of three types. The one-port resistor is an energy dissipating element and the relationship between effort and flow is given by

$$e = Xf \quad (4)$$

where X represents impedance, for example electrical resistance (R) or mechanical damping (D). The one-port capacitor is an energy storing element with a relationship of the form

$$e = (1/X) \int f(t) dt \quad (5)$$

where X here represents electrical capacitance (c) or spring stiffness (k). The one-port inductor is also an energy storing element with a relationship of the form

$$e = X df(t)/dt \quad (6)$$

where X represents electrical inductance (L) or mass (M).

The two-port elements that are of interest in many dynamic problems are the transformer and the gyrator. Both are power conserving and the relationship between the variables is as shown in Table 15.1. The three-port elements are also power conserving elements and are of two types – the 1-junction and the 0-junction. The relationship between the variables is as shown in Table 15.1.

With this background we are now in a position to build models of the air pump using bond-graphs.

4 Model Development

In this section we develop a sequence of models starting from the simplest.

4.1 Model 1

A simple model is obtained by ignoring all energy storage and dissipation elements. The system is viewed as being made of three separate energy (or power) transforming elements. As a consequence the model is given by the schematic representation shown in Figure 15.3. We have discussed each of the three devices in Section 2. The inputs to the model are e_i and i_i and the outputs are p_o and q_o . The model is given by equations (1)–(3) and the following

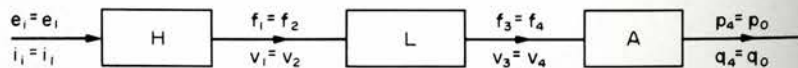


FIGURE 15.3 Schematic representation of Model 1.

equations

$$\left. \begin{aligned} e_1 &= e_i \\ i_1 &= i_i \end{aligned} \right\} \quad (7)$$

$$\left. \begin{aligned} f_2 &= f_1 \\ v_2 &= v_1 \end{aligned} \right\} \quad (8)$$

$$\left. \begin{aligned} f_4 &= f_3 \\ v_4 &= v_3 \end{aligned} \right\} \quad (9)$$

and

$$\left. \begin{aligned} p_o &= p_4 \\ q_o &= q_4 \end{aligned} \right\} \quad (10)$$

From these we obtain the following relationship between the output and the input.

$$\left. \begin{aligned} q_o &= (AL/H)e_i \\ i_i &= (AL/H)p_o \end{aligned} \right\} \quad (11)$$

The reason for writing (11) as indicated above is that in the design e_i (the input voltage) and p_o (the pressure at which air is to be delivered) are specified. The selection of system parameters (given by A , L and H) determine q_o and i_i uniquely. In other words, e_i and p_o are the independent variables (for design purposes) and q_o and i_i are the dependent variables. As no energy is stored or dissipated, we have

$$p_o q_o = e_i i_i \quad (12)$$

The main drawbacks of this model are as follows:

- (i) Since the model ignores all energy dissipative elements it is highly unrealistic.
- (ii) Because of (i), the variable $q_o(i_i)$ changes instantaneously as $e_i(p_o)$ changes; this also is unrealistic.
- (iii) As p_o increases, i_i also increases. Thus, should a blockage occur on the output side, the current drawn (i_i) approaches infinity. This follows because a blockage is equivalent to $p_o \rightarrow \infty$. This is not true, and hence the model is unacceptable.

The bond-graph representation of this model is shown in Figure 15.4. This representation contains more information than the schematic representation shown in Figure 15.3; i.e. causal relationships (indicated by short vertical lines)

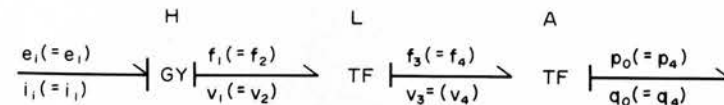


FIGURE 15.4 Bond-graph representation of Model 1.

and flow of power (indicated by half-arrow tips). The advantage of bond-graph representation becomes more noticeable as we improve on this simple model.

4.2 Model 2

This model includes two new features, which are the mass of the magnet and the compliance of the bellows. Both of these are energy storage elements. The effect of including the mass of magnet is that $f_2 \neq f_3$. This follows as the total force generated by the electromagnetic actuator must now equal the force to move the magnet (given by mass times rate of change of velocity) plus the force to operate the lever mechanism. As a consequence, instead of (8) we have*

$$\left. \begin{aligned} f_1 &= f_2 + M dy_2/dt \\ v_2 &= v_1 \end{aligned} \right\} \quad (13)$$

From (1) we see that

$$\left. \begin{aligned} f_2 v_2 &= f_1 v_1 - M v_2 dv_2/dt \\ &= f_1 v_1 - d/dt \{ M v_2^2/2 \} \end{aligned} \right\} \quad (14)$$

This can be interpreted as follows: power generated to drive the lever and bellows ($f_2 v_2$) is equal to the power generated by the electromagnetic actuator ($f_1 v_1$) minus the power used in altering the kinetic energy stored in the mass of magnet.

The effect of the compliance of the bellows is also similar and, as a consequence, instead of (9) we have

$$\left. \begin{aligned} f_4 &= f_3 - K \int v_3 dt \\ v_4 &= v_3 \end{aligned} \right\} \quad (15)$$

where K is the compliance of the bellows.

Thus the overall model is given by equations (1)–(3), (7), (10), (13) and (15) (i.e. it differs from the earlier model in the sense that (8) and (9) are replaced by (13) and (15) respectively). Defining:

$$x_2 = f_3 - f_4 \quad (16)$$

and on manipulating the above-mentioned set of equations, we have

$$q_0 = (AL/H)e_i \quad (17)$$

and

$$i_i = (M/H^2)\{de_i/dt\} + (1/H)\{Lx_2 + LAp_0\} \quad (18)$$

$$dx_2/dt = (KL/H)e_i \quad (19)$$

*We shall omit writing the argument t for notational convenience. Thus, we shall write v_2 instead of $v_2(t)$, and so on.

Equation (17) is the same as the first equation in (11). However, i_i differs, as it is a function of both the derivative and the integral of e_i . The drawbacks of this model are as follows.

- (i) q_0 changes instantaneously with changes in e_i ;
- (ii) if e_i changes suddenly (e.g. a step change), then i_i assumes unbounded values. This does not happen in real life; hence this model is still inadequate and needs to be further modified.

4.3 Model 3

Model 2 was obtained from a system characterization which ignored all energy losses in the system. In contrast, Model 3 is obtained from a modified system characterization which includes a feature to account for one such loss. More specifically, it treats the coil (or the electromagnetic actuator) as having a non-zero resistance R . As a consequence energy is dissipated in the form of heat. The system characterization is otherwise the same as for the previous model. The bond-graph representation for this characterization is given in Figure 15.5.

As a consequence equation (7) gets modified to

$$\left. \begin{aligned} e_1 &= e_i - i_i R \\ i_1 &= i_i \end{aligned} \right\} \quad (20)$$

and the model is given by this and (1)–(3), (10), (13) and (15).

By manipulating these equations (and using x_2 as given by (16)) we have

$$q_0 = ALv_1 \quad (21)$$

$$i_i = (e_i - Hv_1)/R \quad (22)$$

with

$$dv_1/dt = (1/M)\{(H/R)e_i - (H^2/R)v_1 - Lx_2 - LAp_0\} \quad (23)$$

and

$$dx_2/dt = ALv_1 \quad (24)$$

Thus this model overcomes all the drawbacks of Model 1. However, this is still not adequate as it ignores various other features – compressibility, air friction, etc.

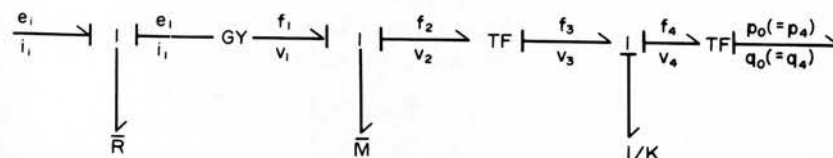


FIGURE 15.5 Bond-graph representation of Model 3.

At this point it is worth noting that the complexity of the underlying mathematical formulation for both Models 2 and 3 is the same in that they each involve two coupled ordinary differential equations. This is in contrast to Model 1, whose underlying formulation is algebraic. As we make the system characterization more detailed, i.e. include more features, the complexity of the underlying formulation used in the model also increases.

4.4 Model 4

The system characterization for this model differs from that for the previous model in that we include the effect of air compressibility. The effect of this is that we have one more energy storage element in the system characterization. As a consequence (10) needs to be modified, for the output flow rate $q_0 \neq q_4$. The modified relationship is given by

$$\left. \begin{aligned} p_0 &= p_4 \\ q_0 &= q_4 - C dp_4/dt \end{aligned} \right\} \quad (25)$$

Thus the complete model is given by (1)–(3), (13), (15), (20) and (25).

On manipulating these equations, we have

$$q_0 = ALv_1 - C dp_4/dt \quad (26)$$

$$i_i = (e_i - H v_1)/R_1 \quad (27)$$

with

$$dx_2/dt = K L v_1 \quad (28)$$

$$dv_1/dt = (1/M)\{(H/R)(e_i - H v_1) - L A p_4 - L x_2\} \quad (29)$$

In this model, if q_0 is held constant, then p_4 must fluctuate with time as v_1 fluctuates. Since $p_0 = p_4$, this implies that both the output pressure and flow rate cannot be held constant. If the output pressure is held constant, then the output flow rate fluctuates and is given by

$$q_0 = ALv_1$$

and i_i is given by (27).

4.5 Model 5

The system characterization for this model includes losses due to air friction resistance and coil resistance. Hence it is an improvement over the previous model. Because of the air friction being included (25) gets modified to

$$\left. \begin{aligned} p_0 &= p_4 - R_0 q_0 \\ q_0 &= q_4 - C dp_4/dt \end{aligned} \right\} \quad (30)$$

where R_0 is the resistance coefficient.

Thus the overall model is given by (1)–(3), (13), (15), (20) and (30). These can be simplified to yield

$$q_0 = (p_4 - p_0)/R_0 \quad (31)$$

$$i_i = (e_i - H v_1)/R_1 \quad (32)$$

with

$$dp_4/dt = (1/C)\{ALv_1 - (p_4 - p_0)/R_0\} \quad (33)$$

$$dx_2/dt = K L v_1 \quad (34)$$

$$dv_1/dt = (1/M)\{(H/R)(e_i - H v_1) - L A p_4 - L x_2\} \quad (35)$$

On comparison with Model 4 we see that the underlying formulation involves three coupled ordinary differential equations.

4.6 Model 6

The system characterization for this model is again an improvement over that for Model 5, as it includes two new features – damping in the bellows and inductance of the coil. The bond-graph representation is given in Figure 15.6. As a consequence (20) and (15) get modified to

$$e_1 = e_i - i_1 R - L_0 di_1/dt \quad (36)$$

$$i_i = i_1$$

and

$$\left. \begin{aligned} f_4 &= f_3 - K \int v_3 dt - B v_3 \\ v_4 &= v_3 \end{aligned} \right\} \quad (37)$$

where L_0 is the inductance of the coil and B the damping coefficient.

The complete model is given (1)–(3), (13), (30), (36) and (37). This set of equations can be rewritten as

$$\left. \begin{aligned} q_0 &= (p_4 - p_0)/R_0 \\ i_i &= i_1 \end{aligned} \right\} \quad (38)$$

with

$$dp_4/dt = (1/C)\{ALv_1 - (p_4 - p_0)/R_0\} \quad (39)$$

$$dx_2/dt = K L v_1 \quad (40)$$

$$dv_1/dt = (1/M)\{H i_1 - L A p_4 - L x_2 - L^2 B v_1\} \quad (41)$$

$$di_1/dt = (1/L_0)\{e_i - H v_1 - R i_1\} \quad (42)$$

The underlying formulation is a set of four coupled first-order ordinary differential equations.

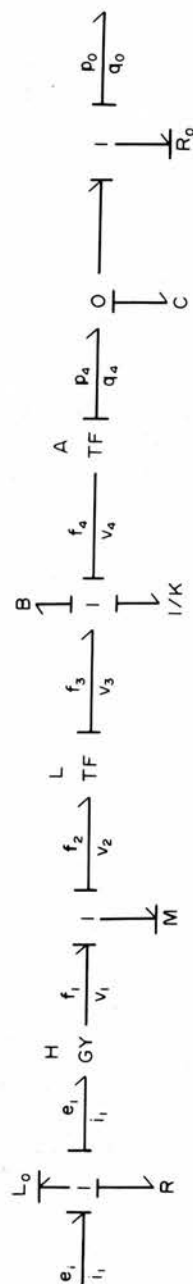


FIGURE 15.6 Bond-graph representation of Model 6.

TABLE 15.2 Relationship between Mathematical Equations of Models 1–6

Model					
1	2	3	4	5	6
2	2	2	2	2	2
3	3	3	3	3	3
7	7	20	20	20	36
8	13	13	13	13	13
9	15	15	15	15	37
10	10	10	25	30	30

4.7 Discussion

Since each model is an improvement over the previous one, Models 1–5 are special cases of Model 6. To illustrate this better, we present the underlying equations of the models in a tabular form in Table 15.2. The arrows indicate the changes resulting from the inclusion of one or more new features.

Because of (4)–(6) the relationships between variables are all linear. This is justified only when changes in the variables are small. When these changes become large, the linear relationships of (4)–(6) are no longer valid and one needs to use non-linear relationships. As a result the complexity of the underlying formulations will increase. Finally, on comparing Model 1 with Model 6, we see that the former uses a static formulation with only three parameters while the latter uses a dynamic one with four coupled first-order linear ordinary differential equations with ten parameters. We could improve further on the last model, but for design purposes it is adequate, for it incorporates all significant components of the system.

5 Analysis

Since the input voltage is the line voltage which is sinusoidal, and the output pressure p_0 a constant, the current drawn (i_i) and the flow rate (q_0) are also sinusoidal. The variables of interest are the amplitudes of i_i and q_0 as functions of model parameters and input line frequency ω .

We start by rewriting the equations in matrix form.

Define $x_1 = p_4$, $x_3 = v_1$, and $x_4 = i_1$. Then (39)–(42) can be rewritten as a matrix differential equation of the form

$$dX/dt = \tilde{A}X + \tilde{B}u \quad (43)$$

where

$$\begin{cases} X^T = [x_1 & x_2 & x_3 & x_4] \\ u^T = [e_i & p_0] \end{cases} \quad (44)$$

$$\tilde{A} = \begin{bmatrix} -(1/R_0 C) & 0 & (AL/C) & 0 \\ 0 & 0 & KL & 0 \\ -(LA/M) & -L/M & L^2 B/M & H/M \\ 0 & 0 & -H/L_0 & -R/L_0 \end{bmatrix} \quad (45)$$

$$\tilde{B} = \begin{bmatrix} 0 & 1/R_0 C \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \quad (46)$$

The analysis can be done either in the time domain or in the frequency domain.

5.1 Time Domain Analysis

The equations given by (43)–(46) can be solved either analytically or computationally to obtain the behaviour of $q_0(t)$ and $i_i(t)$ for specified parameter values. As t becomes large, $q_0(t)$ and $i_i(t)$ reach steady state values if the equations are stable.

We shall consider the following nominal values for the ten parameters of the model:

$$\begin{aligned} H &= 13 \text{ Newtons/amp} \\ L &= 0.58 \\ A &= 1.71 \times 10^{-4} \text{ m}^2 \\ M &= 1.11 \times 10^3 \text{ Newton s}^2/\text{m} \\ R &= 2250 \Omega \\ L_0 &= 3.9 H \\ C &= 18.65 \times 10^{-10} \text{ m}^5/\text{Newton} \\ R_0 &= 3.82 \times 10^5 \text{ Newton-s/m}^5 \\ B_0 &= 0 \text{ (i.e. assumed negligible)} \\ K &= 117 \text{ Newton/m} \end{aligned}$$

The input voltage e_i is sinusoidal with an amplitude of 220 volts and a frequency of 50 cycles/s. The output pressure is assumed to be 100 kiloPascals.

The equation, given by (43)–(46), was integrated from $t = 0$ to 10.0 with the initial conditions assumed zero at $t = 0$. Since the equations are fairly stiff, the integration was done using Gear's variable-step package from the NAG algorithm library. The solution was computed to a relative accuracy of 0.0001 and the computations done on VAX using double precision. The output q_0 and the current drawn i_i are shown in Figure 15.7 for the time interval [7.93, 8.00]. Note that the solutions have not yet reached steady state as the amplitudes are still fluctuating.

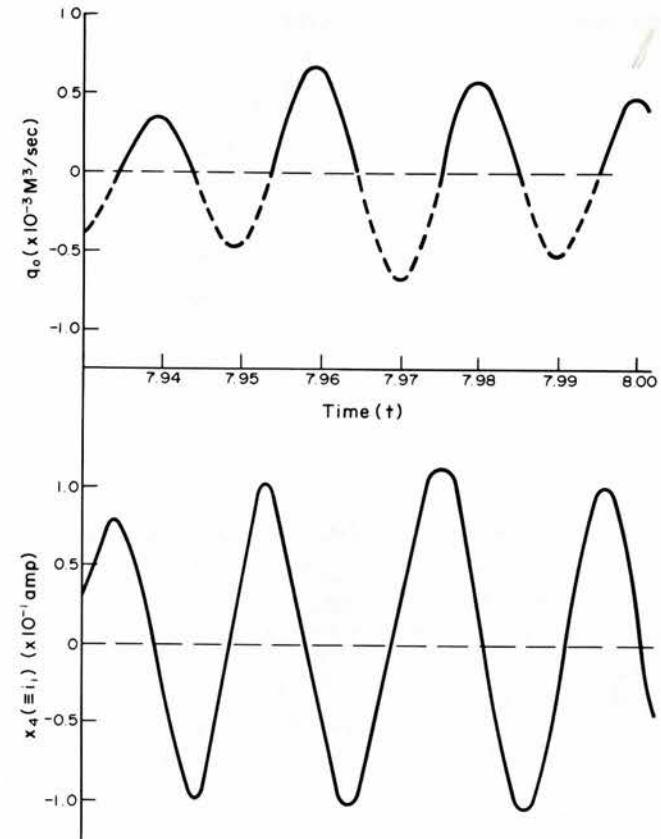


FIGURE 15.7 Plots of $q_0(t)$ and $i_i(t)$.

5.2 Frequency Domain Analysis

Towards this end, let $\hat{X}(s)$ and $\hat{u}(s)$ denote the Laplace transform of $X(t)$ and $u(t)$. From (43) we have

$$\hat{X}(s) = (sI - \tilde{A})^{-1} \tilde{B} \hat{u}(s) \quad (47)$$

Since $p_4(t) = x_1(t)$, we have

$$p_4(t) = x_1(t) = \tilde{C} X(t) \quad (48)$$

with

$$\tilde{C}^T = [1 \ 0 \ 0 \ 0] \quad (49)$$

From (38), we have

$$\hat{q}_0(s) = \{\tilde{C}^T \hat{X}(s) - \hat{p}_0(s)\} / R_0 \quad (50)$$

where $\hat{q}_0(s)$ and $\hat{p}_0(s)$ are the Laplace transforms of $q_0(t)$ and $p_0(t)$ respectively.

After some simplification, we can re-write (50) as

$$\hat{q}_0(s) = \frac{1}{R_0 L_0} \frac{N_1(s)}{D_1(s)} \hat{e}_i(s) + \frac{1}{R_0} \left\{ \frac{N_2(s)}{(R_0 C) D_1(s)} - 1 \right\} \hat{p}_0(s) \quad (51)$$

where

$$N_1(s) = s a_{13} a_{34} \quad (52)$$

$$N_2(s) = s^3 + s^2 \{-a_{33} - a_{44}\} + s \{a_{33} a_{44} + a_{34} a_{43} - a_{23} a_{32}\} + a_{23} a_{44} \quad (53)$$

$$D(s) = s^4 + s^3 \{-a_{11} - a_{33} - a_{44}\} + s^2 \{a_{11} a_{33} + a_{11} a_{44} - a_{32} a_{23} + a_{13} a_{31}\} + s \{-a_{11} a_{33} a_{44} - a_{11} a_{34} a_{43} + a_{23} a_{32} a_{44} - a_{44} a_{13} a_{31}\} + \{-a_{11} a_{23} a_{32} a_{44}\} \quad (54)$$

(Note: a_{ij} ($1 \leq i, j \leq 4$) are the elements of matrix $\tilde{A}$.)

Using $s = jw$ with $w = 2\pi f$, we can study the behaviour of $N_1(s)/D_1(s)$ as f varies. Since $N_1(s)/D_1(s)$ is complex, it consists of a real part and an imaginary part. Defining GAIN as the magnitude of this complex quantity, we have GAIN as a function of frequency f . Good design requires that GAIN be maximum at $f = 50$, implying that the pump develops maximum output flow rate at $f = 50$. The plot of GAIN versus f , for the nominal values mentioned earlier, is shown by curve A in Figure 15.8. Note that GAIN is maximum at $f = 27$.

By changing the lever ratio from 0.58 to 0.68, GAIN was re-evaluated as a function of f . The plot is shown by curve B in Figure 15.8. Note, the peak of GAIN has shifted from 27 to 35. On the other hand, if A is doubled, then the

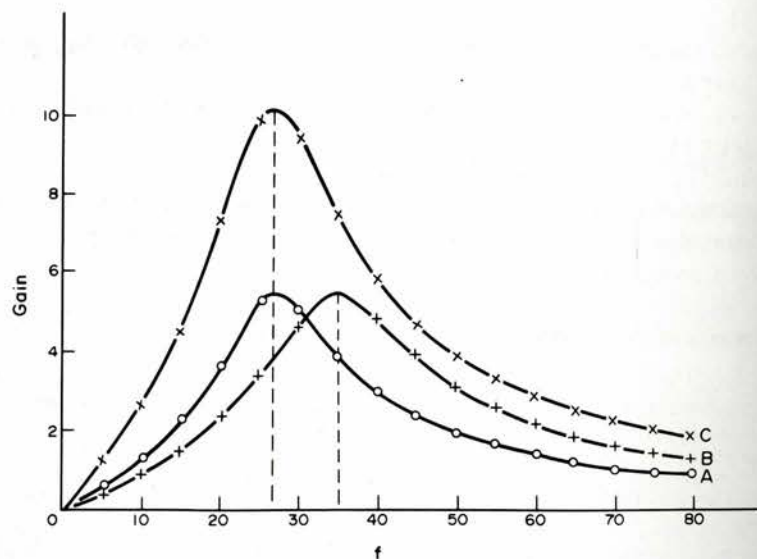


FIGURE 15.8 Plot of gain vs frequency.

plot of GAIN versus f is as shown by curve C in Figure 15.8. In this case, the peak has increased but it occurs at the old frequency.

This type of analysis is useful in selecting the components of the system so that it yields the specified value for GAIN at the specified frequency.

The analyses indicate that the nominal values selected for the parameter of the model (or equivalently, the characteristics of the different components) are not the best, and that these would need to be altered to achieve a peak for GAIN at $f = 50$.

6 Conclusions

In this chapter we have discussed a design problem where the mathematical model plays an important role in the engineering task of designing. We could have transformed the problem to an optimization problem by defining the optimization criterion as the maximization of GAIN at $f = 50$. Viewed this way we have a constrained static optimization problem, since GAIN is related to the parameters by an algebraic equation given by (51). However, our aim has been to illustrate the iterative nature of model building: starting from the simplest model and increasing the complexity till an adequate model of least complexity is obtained.

Notes and References

Our presentation of the bond-graph approach to the modelling of electrical, mechanical and pneumatic systems has been very terse. For further details, see [1]–[3].

The six models presented are due to Martens and Bell [4]. They give the bond-graph representation for all the six models.

The variables x_1 , x_2 , x_3 and x_4 in the final model have physical dimensions. By scaling them properly we can rewrite (43) in a non-dimensional form and overcome the stiffness of the equations.

The analysis of linear models of the form given by (43) can be found in most books on linear system theory. See, for example, [5]. The evaluation of GAIN was done using packages from [6].

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Forecasting Airline Passenger Growth

1 Introduction

Growth in the number of airline passengers is of great interest to airline operators and to planners responsible for developing airports. The importance of forecasts to airline operators is two-fold. In the short term it allows for more efficient scheduling, and in the long term it guides the expensive planning decisions regarding purchase of new planes. If decisions are based on poor forecasts, the economic viability of the airline operator is at stake.

In this chapter we look at the problem of building mathematical models to produce forecasts of growth in the number of airline passengers. We commence with a system characterization relevant for model building in Section 2. A comprehensive model incorporating all the relevant variables is of limited use due to problems associated with the data needed for estimation and validation; instead we shall use the "black-box" approach. The advantage of this is that the model is built and validated using only the available data (namely, the monthly figures for airline passengers). The approach to modelling is discussed in Section 3, where we also give the data that will be used for model building and validation. In Section 4 we carry out some preliminary analysis of the data to decide on the most suitable mathematical formulation for modelling. Since the modelling is highly data-dependent we briefly discuss this aspect in Section 5. In Section 6 we examine the problem of estimating model parameters. In Section 7 we present a sequence of models leading to an adequate one. In Section 8 we discuss some extensions and possible refinements.

2 System Characterization

In this section we examine the relevant variables which affect the growth in the number of airline passengers and other factors such as time interval for aggregation and the appropriate framework for modelling.

2.1 Variables and Relationships

Since we are interested in aggregated numbers, let N_i represent the number of passengers flying in the interval $t = i\Delta$ to $(i + 1)\Delta$ where Δ is specified. We shall discuss the choice of Δ later on. N_i could represent the number of passengers

- (i) travelling within a certain geographical region; or
- (ii) travelling by a certain airline carrier; or
- (iii) travelling within and moving out of a certain geographical area.

What N_i represents depends on the need of the forecaster. For this case study N_i represents the number of airline passengers either moving into or out of the United Kingdom (U.K.).

N_i depends on many other variables. Some of the important ones are:

- (i) cost of travel (e.g. average cost/km);
- (ii) the quality of service relative to other modes of travel;
- (iii) advertising;
- (iv) the general state of the national economy.

Some of these in turn might depend on other variables – for example, the price of aviation fuel and the financial state of the airline operator.

The relationships between the variables can be fairly involved. As an example, the number of passengers carried depends on advertising, which in turn depends on the profitability of the airline; finally, the profitability in turn depends on the number of passengers carried. The dependence involves varying time lags which are difficult to quantify. Similarly, it is difficult to quantify certain variables – for example, quality of service – in a meaningful way.

This suggests that a "black-box" approach is the most appropriate, and we discuss this in the next section.

2.2 Interval for Aggregation

Since the forecasts of interest are the aggregated values, the choice of the time interval over which the number of passengers is to be aggregated is important. We represented this interval by the symbol Δ in our earlier characterization.

If Δ is large, then we have a coarse description, since the aggregation is done over a long interval. As Δ gets smaller the description becomes finer. The choice of Δ is part of the art aspect of modelling. We shall choose Δ to equal 1 month for the following two reasons.

- (i) statistics for passengers carried are usually compiled on a monthly basis; and
- (ii) smaller Δ (say 1 week) is too fine and of limited use.

For long-term planning one might choose Δ equal to 3 months or 6 months, or even a year.

2.3 Deterministic vs Stochastic

Since N_i is affected by many variables, some of which change in an uncertain manner, the most appropriate framework for characterizing N_i is the stochastic framework. The modelling of N_i involves a stochastic formulation with uncertainty characterized explicitly. The variables representing uncertainty can also be viewed as representing the cumulative effect of some of the relevant variables ignored in the modelling.

3 The Black-box Approach

The "black-box" approach to modelling that we will follow is to characterize N_i solely in terms of its previous values (i.e. N_{i-j} , $j \geq 1$) and through an uncertain (or random) sequence W_j ($j \leq i$). The model is given by a mathematical formulation which relates N_i to its previous values and the W_j ($j \leq i$) sequence. The formulation is selected on an *ad-hoc* basis and revised based on the fit between the model output and the historical data available. Thus, the modelling can be viewed as a "data-dependent" one. The precise details of the mathematical formulation that we will be using will be discussed in Section 5, after we have examined the data available for modelling and estimation. The modelling approach that we will be taking is called "stochastic time series modelling" and often the word stochastic is ignored and the term used is "time series modelling". This formulation was discussed in some detail in Section 7.3 of Chapter 7.

The data we will be using for modelling are given in Table 16.1. This shows the monthly aggregates for the number of airline passengers for the U.K., obtained from the monthly statistics published by the government. The data cover the period January 1966–February 1985, and we regard January of 1965 to correspond to $i = 1$. As a result the data available for modelling and validation are given by n_i , $1 \leq i \leq I$ with $I = 230$.*

We are interested in obtaining forecasts for the period March 1985–December 1988; in other words, obtaining estimates of N_i for $231 \leq i \leq 264$.†

*We follow the standard convention for stochastic variables – i.e. upper-case letters represent the variables and lower-case letters represent the realized values. Thus N_i represents the random variable and n_i the observed (or realized) value.

†Rather than model N_i , we model N_i scaled by a factor of 10^{-6} . We shall henceforth use N_i to represent this scaled variable. As a result we would need to scale model forecasts and variances by 10^6 and 10^{12} , respectively, to obtain the true values.

4 Analysis of the Historical Data

A plot of the historical data of Table 16.1 is given in Figure 16.1, and reveals the following:

- (i) the data can be viewed as consisting of a deterministic component and a stochastic component;
- (ii) the deterministic component consists of a trend (or growth) component and a seasonal component;

TABLE 16.1 Historical Data for Airline Passenger Growth (10^6)

Year	Data					
1966	0.6090	0.5496	0.7225	0.9616	1.0948	1.4076
	1.6092	1.5689	1.3546	0.8862	0.6105	0.6833
1967	0.6519	0.5878	0.8539	0.9253	1.1213	1.3201
	1.5517	1.5968	1.4496	0.9690	0.6335	0.6575
1968	0.6402	0.6024	0.7942	0.9939	1.0515	1.2692
	1.4888	1.5567	1.4016	0.9563	0.7001	0.7687
1969	0.7121	0.6265	0.8720	1.0125	1.2084	1.3536
	1.5669	1.6417	1.4698	1.0885	0.8142	0.8492
1970	0.7866	0.7323	1.0057	1.0957	1.2596	1.3408
	1.5847	1.6539	1.5317	1.1299	0.8467	0.8991
1971	0.7543	0.7643	0.9865	1.2122	1.2937	1.4813
	1.6761	1.6916	1.6115	1.2276	0.8250	0.9342
1972	0.8970	0.7923	1.0760	1.2495	1.4566	1.5581
	1.7049	1.7390	1.7785	1.4007	1.0239	1.0904
1973	1.0214	0.9155	1.2193	1.4605	1.5469	1.6878
	1.8305	1.8793	1.8930	1.4976	1.2114	1.2011
1974	1.1066	0.9873	1.1860	1.3993	1.3434	1.5904
	1.7031	1.7424	1.7901	1.3910	1.0667	1.0895
1975	1.0342	0.8976	1.1930	1.2234	1.3728	1.4647
	1.7272	1.8009	1.7546	1.5015	1.1217	1.1409
1976	1.1119	1.0150	1.2966	1.4164	1.4916	1.6686
	1.7734	1.8018	1.8135	1.5299	1.2304	1.2366
1977	1.7337	1.1013	1.4106	1.1071	1.5193	1.7188
	1.8541	1.6884	1.5820	1.3719	1.2766	1.2795
1978	1.2490	1.1498	1.5474	1.5851	1.7619	1.9041
	2.1154	2.1080	2.0637	1.8177	1.5152	1.4168
1979	1.2628	1.2367	1.5905	1.8749	1.9859	2.1109
	2.3573	2.4409	2.2805	2.0581	1.5985	1.5130
1980	1.4713	1.4042	1.7318	1.7910	1.8944	2.0760
	2.2716	2.3677	2.1611	1.9428	1.5413	1.5378
1981	1.4905	1.3706	1.6129	1.8020	1.7615	1.8558
	2.1356	2.2615	2.1572	1.9283	1.5705	1.4140
1982	1.4971	1.3207	1.5942	1.7416	1.7356	1.8747
	2.1364	2.0586	1.9945	1.7847	1.4396	1.4304
1983	1.3962	1.2560	1.6144	1.6364	1.7379	1.8764
	2.0450	2.0074	2.0417	1.8177	1.4822	1.4733
1984	1.4428	1.3594	1.6228	1.8185	1.9519	2.1055
	2.2425	2.2569	2.2878	2.0798	1.7389	1.6506
1985	1.6115	1.4765				

Source: Reference [1]

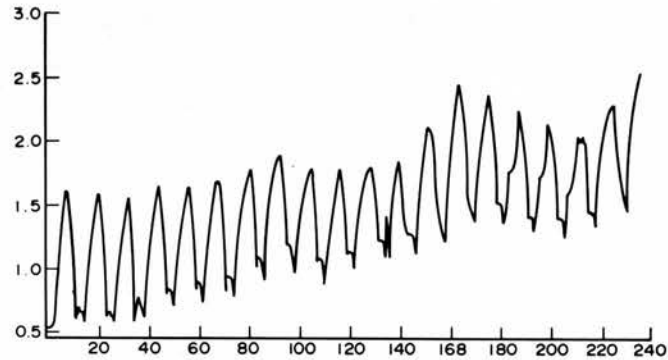


FIGURE 16.1 Monthly figures for airline passengers.

- (iii) the trend component is linear in time and the seasonal component exhibits a periodic pattern with a period of 12 months.

The reasons for the linear trend are: population growth, air travel becoming relatively cheaper than other modes of travel, and the increase in the general standard of living which allows more time for leisure. The periodic pattern is due to seasonal factors – passenger numbers increasing in the summer months, which coincide with the holiday season as well as being the best time to travel. The stochastic component is due to various uncertainties which cause random variations.

Thus, N_i can be viewed as comprising the following components:

$$N_i = D_i + P_i + W_i \quad (1)$$

where D_i and P_i represent the deterministic trend and periodic components, and W_i the stochastic component.

If we assume that the deterministic trend is linear, D_i is of the form

$$D_i = a + bi \quad (2)$$

By differencing, we have

$$D_i - D_{i-1} = b \quad (3)$$

and

$$(D_i - D_{i-1}) - (D_{i-1} - D_{i-2}) = 0 \quad (4)$$

i.e. the trend component in N_i can be eliminated.

Motivated by the need for a compact notation, we define two operators – the backward difference operator and the backward shift operator. The k th-order backward difference operator ∇_k , $k \geq 1$, is defined as

$$\nabla_k N_i = N_i - N_{i-k} \quad (5)$$

and the k th-order backward shift operator B_k , $k \geq 1$, is defined as

$$B_k N_i = N_{i-k} \quad (6)$$

When $k = 1$ we use ∇ and B instead of ∇_1 and B_1 , and the two are related by the relation

$$\nabla = 1 - B \quad (7)$$

As a result (3) and (4) can be rewritten as

$$\nabla D_i = b \quad (8)$$

and

$$\nabla^2 D_i = 0 \quad (9)$$

where ∇^j is the operator ∇ applied j times.

Since the periodic component has a period of 12 months, if we assume that P_i is of the form

$$P_i = A \sin(\pi i/6 + Q) \quad (10)$$

where A and Q are constants, then taking a twelfth-order difference we have

$$\nabla_{12} P_i = (1 - B_{12})P_i = 0 \quad (11)$$

Thus the periodic component can be removed by such a differencing.

With this background we now define two new time series – Y_i and Z_i – which are as follows:

$$Y_i = \nabla N_i, \quad i \geq 2 \quad (12)$$

and

$$Z_i = \nabla_{12} Y_i, \quad i \geq 14 \quad (13)$$

Note that in terms of the backward shift operator (12) and (13) can be written as

$$Y_i = (1 - B)N_i, \quad i \geq 2 \quad (14)$$

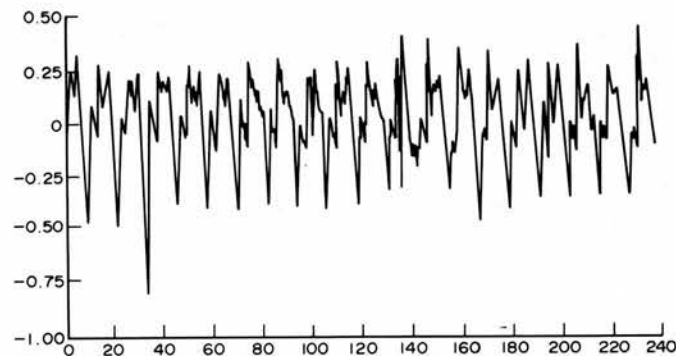
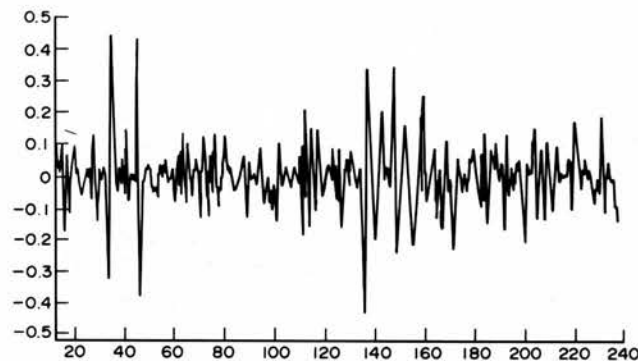
and

$$Z_i = (1 - B)(1 - B_{12})N_i, \quad i \geq 14 \quad (15)$$

We can view Y_i as the time series obtained by the removal of the linear trend from N_i , and Z_i as the time series obtained by the removal of the linear trend and the periodic component. The plots of y_i and z_i are given in Figures 16.2 and 16.3, respectively. Note that z_i is fluctuating about a mean value $\bar{z} = -0.00131$, obtained by the expression

$$\bar{z} = \sum_{i=14}^{230} z_i / 216 \quad (16)$$

Since $\bar{z}$ is very close to zero, we can ignore it. We assume that the Z_i series is

FIGURE 16.2 Plot of y_i vs i (trend removed).FIGURE 16.3 Plot of z_i and i (trend and seasonality removed).

weakly stationary and ergodic.* As a result, estimates of the autocorrelations of Z_i can be obtained from the historical values of z_i , $i \geq 1$. Let $v(k)$ represent the autocovariance of lag k , i.e.

$$v(k) = E[Z_i Z_{i+k}] \quad (17)$$

Then, $\hat{v}(k)$, an estimate of $v(k)$, can be obtained by the relation

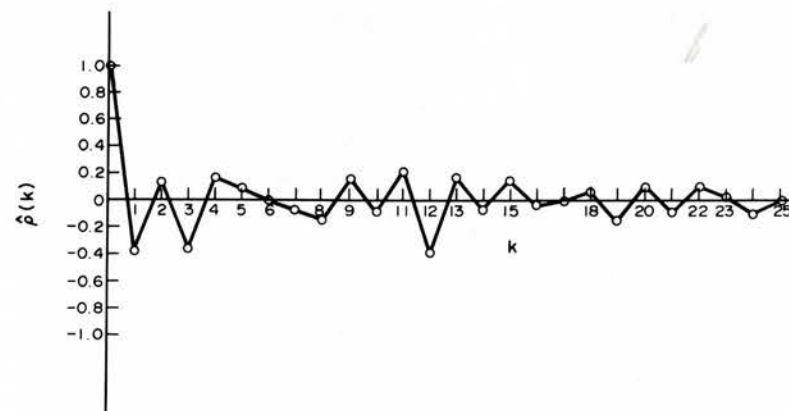
$$\hat{v}(k) = \sum_{i=14}^{230-k} (z_{i+k} - \bar{z})(z_i - \bar{z}) / (216 - k) \quad (18)$$

Rather than $v(k)$, we shall deal with the autocorrelation $\rho(k)$ given by

$$\rho(k) = v(k)/v(0) \quad (19)$$

*Weakly stationary implies that the mean $E\{Z_i\}$ does not change with i and the autocovariance $E\{Z_i Z_{i+k}\}$ is a function of only k . Ergodicity implies that the ensemble averages can be obtained by time averaging - e.g.

$$E\{z_i\} = \lim_{N \rightarrow \infty} \sum_{i=1}^N Z_i / N, \text{ and so on.}$$

FIGURE 16.4 Plot of $\hat{\rho}(k)$ vs k .

Let $\hat{\rho}(k)$ represent the estimated value of $\rho(k)$. A plot of $\hat{\rho}(k)$, $0 \leq k \leq 25$, is given in Figure 16.4. Note that $\hat{\rho}(k)$ is significantly different from zero for $k > 0$, indicating that Z is a correlated sequence. (Since $\rho(k) = \rho(-k)$, we shall confine our discussion to $k > 0$.)

The above statement, that Z_i is a correlated sequence, is based on visual assessment. A rigorous procedure is needed to establish this fact. This can be done by a hypothesis-testing procedure discussed in the next section. We omit details of the tests; these can be found in the reference cited in the Notes at the end of the chapter.

4.1 A Test for Serial Correlation

Suppose that Z_i is an uncorrelated Gaussian sequence with zero mean and finite variance. Let $\hat{\rho}(k)$, $1 \leq k \leq K$ be the sample autocorrelation obtained using the available data z_i , $14 \leq i \leq 216$. Then, the variable STA given by

$$\text{STA} = 216 \sum_{k=1}^K \hat{\rho}^2(k) \quad (20)$$

is distributed according to a χ^2 distribution with K degrees of freedom.

We can use the above result to test the null hypothesis that Z_i is an uncorrelated sequence. Using the values of $\hat{\rho}(k)$ given in Figure 16.4, we have

$$\text{STA} = 135.583 \quad (21)$$

and $K = 25$. From the tables of χ^2 distribution with 25 degrees of freedom, the null hypothesis, that Z_i is an uncorrelated Gaussian sequence with zero and finite variance, can be accepted as being true with 95 per cent confidence only if STA is less than 37.7. Since the computed STA is greater than 37.7 we must

reject the null hypothesis. In other words we must accept the alternative hypothesis that Z_i is a correlated sequence.

5 Modelling Methodology

We first build a stochastic model to describe the changes in Z_i using the historical data available. Once this is done we obtain forecasts $\hat{Z}_i$ of Z_i for $i > 230$ from the model. Using this in (15) we then obtain the forecast $\hat{N}_i$ for $230 < i < 264$. Note that the forecasts cover the period March 1985 to December 1987.

5.1 Modelling the Z Sequence

Since we have assumed that the Z_i sequence is a Gaussian ergodic process, the mathematical formulation most suited for modelling Z_i is an autoregressive moving average (ARMA) formulation. We discuss two different structures for the model formulation.

STRUCTURE I

The structure of the model formulation is given by the relation

$$Z_i + \sum_{j=1}^l \alpha_j Z_{i-j} = V_i + \sum_{j=1}^m \beta_j V_{i-j} \quad (22)$$

subject to the following conditions:

- (C1) l and m are non-negative integers with at least one of them being non-zero;
 (C2) the roots of the following two polynomial equations

$$Q_1(x) = x^l + \sum_{j=1}^l \alpha_j x^{l-j} = 0$$

and

$$Q_2(x) = x^m + \sum_{j=1}^m \beta_j x^{m-j} = 0 \quad (23)$$

all lie strictly inside the unit circle.

- (C3) V_i is a sequence of independent and identically distributed Gaussian random variables with zero mean and variance σ^2 .

Some comments are appropriate at this stage.

- (i) If both l and m are zero, then Z_i is an independent sequence and hence not appropriate for modelling.
 (ii) The root condition ensures that Z_i is stationary and ergodic.

- (iii) Since the formulation is linear, and V_i a Gaussian sequence, Z_i is also a Gaussian sequence.
 (iv) The parameters are given by the set

$$\Theta = \{l, m; \alpha_j, 1 \leq j \leq l; \beta_j, 1 \leq j \leq m; \sigma^2\} \quad (24)$$

i.e. the total number of unknown parameters is $(l + m + 3)$. The parameters are constrained – that is, $\alpha_j, 1 \leq j \leq l$ and $\beta_j, 1 \leq j \leq m$ must ensure that the root condition (C2) is satisfied; l and m satisfy condition (C1), and σ^2 by definition must be positive.

STRUCTURE II

This is a slightly more general formulation to model Z_i and is given by the following relation:

$$Z_i + \sum_{j=1}^{l'} a_j Z_{i-j} = W_i + \sum_{j=1}^{m'} b_j W_{i-j} \quad (25)$$

with W_i given by

$$W_i + \sum_{j=1}^l \alpha_j W_{i-j} = V_i + \sum_{j=1}^m \beta_j V_{i-j} \quad (26)$$

subject to the following conditions:

- (C1') l, m, l' and m' being non-negative integers with either l or m being positive;
 (C2') the roots of the polynomial equation given by (23) and of the following equations

$$Q_3(x) = x^{l's} + \sum_{j=1}^{l'} a_j x^{(l'-j)s} = 0$$

and

$$Q_4(x) = x^{m's} + \sum_{j=1}^{m'} b_j x^{(m'-j)s} = 0 \quad (27)$$

all lie inside the unit circle.

- (C3') Same as in (C3).

This model formulation contains more parameters than the model formulation discussed earlier. The additional parameters are given by the set

$$\Phi = \{s; l', m'; a_j, 1 \leq j \leq l'; b_j, 1 \leq j \leq m'\} \quad (28)$$

The advantage of this formulation is that it allows for correlation at lags which are multiples of s . Note that by setting l' and m' to zero this formulation reduces to the earlier formulation. We assume $s = 12$.

5.2 Modelling Procedure

We assume that the model formulation is given by (25) and (26) subject to constraints (C1')–(C3'). We divide the model parameters into two sets as follows:

$$\Theta_1 = \{l, m, l', m'\} \quad (29)$$

and

$$\Theta_2 = \{\alpha_j, 1 \leq j \leq l; \beta_j, 1 \leq j \leq m; a_i, 1 \leq i \leq l'; b_j, 1 \leq j \leq m' \text{ and } \sigma^2\} \quad (30)$$

The first set characterizes the order of the model formulation. The model complexity increases as the values assigned to the parameters of this set increase. The second set depends on the first set and represents the coefficients of the model formulation and the variance of the random input.

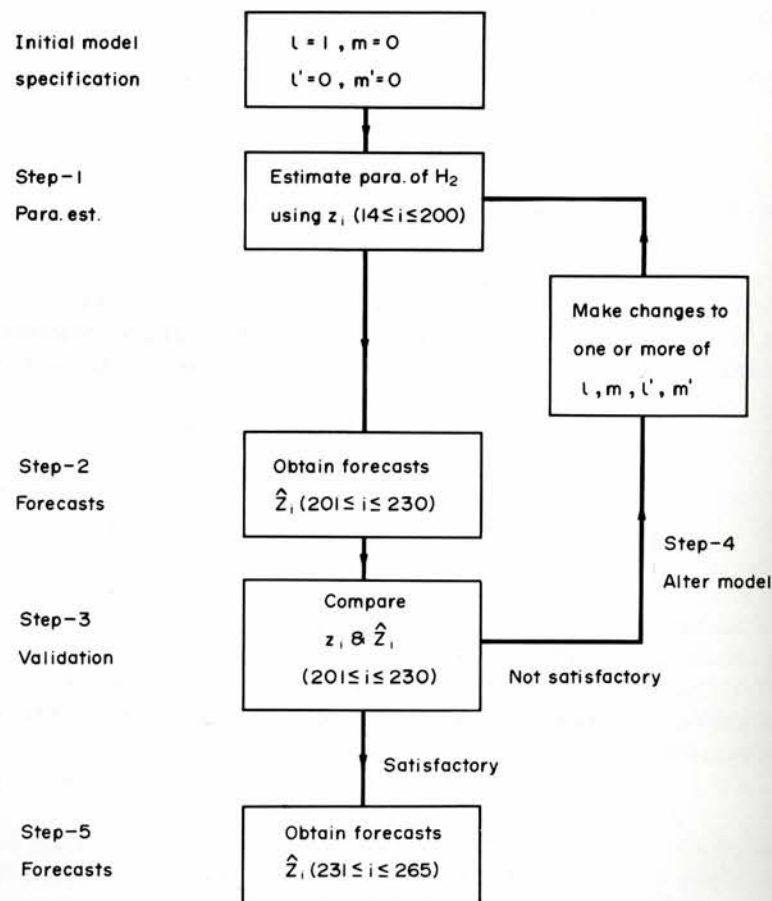


FIGURE 16.5 Model building procedure.

The modelling is done in an iterative manner shown in Figure 16.5. Essentially it consists of the following four steps.

Step 1: Estimate the parameters of set Θ_2 . The estimation is done using z_i , $14 \leq i \leq 200$. The details of the estimation procedure will be discussed in the next subsection.

Step 2: Using the estimated values, forecasts $\hat{Z}_i$ are obtained for $201 \leq i \leq 230$. This is done by using (25) and (26) and assuming zero values for V_i , $201 \leq i \leq 230$.

Step 3: The forecast values $\hat{Z}_i$ are compared with the historical data z_i for $201 \leq i \leq 230$. A validation criterion is used to decide whether the model under consideration is adequate or not. We discuss this aspect in some detail in the next section.

Step 4: If the validation test in Step 3 implies inadequacy of the model, the model is altered by changing the values assigned to one or more of the parameters of set Θ_1 and the procedure repeated.

Step 5: This step is executed only after the validity of the model has been established, and is done in a manner similar to Step 3 to obtain the forecasts for the period $231 \leq i \leq 265$.

The iterative procedure is initiated by an initial specification for the parameters of set Θ_1 . We start with the simplest specification:

$$l' = m' = m = 0 \text{ and } l = 1$$

We first consider only varying l and m (in other words, Structure I model formulation) and later varying either l' and/or m' from zero (in other words, Structure II model formulation). The reason for this is that our aim is to build an adequate model of least complexity.

We use the time series packages from the NAG library to execute all the steps, except Step 4. Step 4 is done manually, using a simple strategy of altering only one parameter of the set Θ_1 at each stage of the iteration. We omit the details of the program, as discussing it will cause a significant digression from the main theme: that of building an adequate model. Further discussion of the NAG package can be found in the Notes at the end of the chapter.

It is worth noting that we have divided the available data z_i , $1 \leq i \leq 230$, into two parts. The first part, comprising $1 \leq i \leq 200$ (or approximately 16 years), is used for parameter estimation and the second part, comprising $201 \leq i \leq 230$ (or $2\frac{1}{2}$ years), is used for model validation. This is done to ensure that the data used for validation are different from these used for parameter estimation. The breakpoint in the data (which corresponds to $i = 200$) is arbitrary.

5.3 Parameter Estimation

The parameter estimation in Step 1 can be done using more than one method. The package in the NAG library estimates the parameters by the method of

maximum-likelihood. As discussed in Chapter 10, Section 4, this method provides statistically the most efficient estimates of parameters. In addition, the package provides extra statistical results useful for the purpose of validation.

The maximum-likelihood estimates of the parameters of the set Θ_2 (except σ^2) are obtained by minimizing J given by

$$J = \sum_{i=14}^{200} \hat{v}_i^2 \quad (31)$$

where $\hat{v}_i, 14 \leq i \leq 200$, are given by

$$\hat{v}_i + \sum_{j=1}^m \beta_j \hat{v}_{i-j} = \hat{w}_i + \sum_{j=1}^l \alpha_j \hat{w}_{i-j} \quad (32)$$

and $\hat{w}_i, 14 \leq i \leq 200$, are given by

$$\hat{w}_i + \sum_{j=1}^{m'} b_j \hat{w}_{i-sj} = z_i + \sum_{j=1}^{l'} a_j z_{i-js} \quad (33)$$

with $s = 12$.

The computer package starts with some nominal value for the parameters of the set Θ_2 . For a specified parameter value it computes J using (31) by solving for $\hat{v}_i$ using (32) and (33). In other words, it computes J as a function of the parameters being estimated. Using an iterative optimization scheme it computes the optimal value of the parameters which minimize J , at the same time ensuring that the root constraints are not violated. The optimizing values are the maximum likelihood estimates. The estimate $\hat{\sigma}^2$ of σ^2 is obtained by the relation

$$\hat{\sigma}^2 = J/186 \quad (34)$$

where J is evaluated using the maximum-likelihood estimates.

6 Model Validation

To establish the adequacy of a given model (in other words, to validate a given model) one needs to define a suitable criterion or test. Validity of the model can be established by

- (i) checking the validity of the underlying assumptions;
- (ii) goodness-of-fit between the model and the actual data;
- (iii) combination of (i) and (ii).

In this section we will discuss (i) and (ii).

6.1 Validation Based on Model Assumption

Since we assumed that V_i is an uncorrelated Gaussian sequence, if the model is an adequate representation then the sequence $\hat{v}_i, 14 \leq i \leq 200$, can be viewed as

estimates of V_i . Thus the validity of the model can be established by checking for the lack of correlation in the $\hat{v}_i$ sequence.

Towards this end, we define the following statistics:

$$STA = 186 \sum_{k=1}^K \hat{\rho}^2(k) \quad (35)$$

where $\hat{\rho}(k)$ is the estimated autocorrelation coefficient of lag $k, 1 \leq k \leq K$, using the sequence $\hat{v}_i, 14 \leq i \leq 200$. If $\hat{v}_i$ is a realization of an independent sequence, then STA is approximately distributed according to a χ^2 distribution with $\{K - (l + m + l' + m')\}$ degrees of freedom (see Box and Jenkins [2], p. 291). Thus, by choosing a sufficiently large K , we can devise a test for validating the model (or establishing adequacy) as follows.

Compute STA using (35) and test whether the computed value is below a number $\bar{L}$ obtained from the tables for χ^2 distribution with $\{K - (l + m + l' + m')\}$ degrees of freedom for a specified confidence limit. If STA is bigger than $\bar{L}$, then we reject the model as being inadequate. If not (i.e. STA is less than $\bar{L}$), then we can either accept the model as being adequate or subject the model to further testing. We will use $K = 25$ and 95 per cent confidence level for testing.

An alternative test for model adequacy is as follows. If $\hat{v}_i$ is a realization of an independent sequence with zero mean, then $\hat{\rho}_v(k)$ estimated using 186 data points is distributed (approximately) according to a Gaussian distribution with zero mean and variance roughly equal to $1/186$. Hence, in this case $\hat{\rho}(k)$ must lie within $\pm 3/\sqrt{186}$ if the assumptions are valid. Thus, we accept a model as being adequate if $\hat{\rho}_v(k), 1 \leq k \leq K$ ($K = 25$) lie inside this band; otherwise we reject the model.

6.2 Validation Based on Forecasting

Since the aim of the model is to forecast, a suitable test is one which compares the goodness-of-fit between the model prediction and the historical data. This is possible in our case, since we have data $z_i, 201 \leq i \leq 230$, which we set aside for this purpose.

The forecast, or predictive, ability can be defined through various measures. One which we shall use is the sum of error squares given by

$$ESQR = \sum_{i=201}^{230} (\hat{Z}_i - z_i)^2 \quad (36)$$

where $\hat{Z}_i$ is the forecast values obtained from the model.

A test which we will use for deciding the validity of a model is as follows. Accept the model as an adequate representation if $ESQR/30 \leq \delta$, otherwise reject the model. Since the model is stationary, $\delta > \sigma_z^2$ where σ_z^2 is the variance of Z_i . For our test we shall use $\delta = g\sigma_z^2$, where g is a positive constant greater than one. Since σ_z^2 is unknown, we use an estimate obtained from the historical data. This yields a value 0.01512 for σ_z^2 . We shall choose $g = 3$. Note that as we make g smaller (bigger) the test becomes more (less) stringent.

7 Models Tested

The methodology discussed in Section 5 was used to build and test a variety of models with $l' = m' = 0$ (i.e. Structure I formulations) for all possible combinations of l and m with $(l + m) = 1, 2, 3, 4, 5$ and 6 . Table 16.2 shows the computer output for a sample of the models tested. It gives the order of l and m ; the statistics of the residuals – viz. $\hat{\sigma}^2$, STA and the degrees of freedom $(25 - l' - m' - l - m)$; the statistics of the forecast performance ESQR; and finally, $\bar{L}$ obtained from the tables of χ^2 distribution for the purposes of validation. For all the models tested, STA is greater than $\bar{L}$; hence no model can be accepted as being adequate. The reason for this can be seen from Figure 16.4; it shows that $\hat{\rho}^2(k)$ is significant for $k = 12$ and 24 . In other words there are correlations of lag 12, the period for the seasonality in the data. This suggests that one should use models involving Structure II formulation as opposed to Structure I formulation.

A variety of models were built and tested for all possible combinations of $l' + m' = 1$ and 2 and $l + m = 1, 2, 3, 4, 5$ and 6 . For some combinations the package failed to yield estimates, due to its inability to find a stationary model to fit the data. These combinations were ignored. Table 16.3 shows the computer output for a sample of the successful models tested. Models MO3001 and MO4001 yielded the best results. For both models, STA is less than L as well as ESQR/30 being less than $3\hat{\sigma}_z^2$, indicating that we accept both the models as being adequate. Note that model MO3001 has a slightly smaller value for STA and a slightly bigger value for ESQR when compared with the corresponding statistics for model MO4001. Since the differences

TABLE 16.2 Computer Results for Model Structure I

Model	l	m	STA	D.F.	$\hat{\sigma}^2$	ESQR	$\bar{L}$
MO1000	1	0	93.9812	24	0.01288	4.40985	36.4
MO2000	2	0	92.2716	23	0.01284	4.31495	35.2
MO3000	3	0	49.1419	22	0.01095	2.87651	33.9
MO4000	4	0	44.3280	21	0.01071	2.54135	32.7
MO5000	5	0	39.8483	20	0.01048	3.04159	31.4
MO3100	3	1	46.9353	21	0.00977	3.65098	32.7

TABLE 16.3 Computer Results for Model Structure II

Model	l	m	l'	m'	STA	D.F.	$\hat{\sigma}^2$	ESQR	$\bar{L}$
MO1001	1	0	0	1	49.2002	23	0.00806	1.15245	35.2
MO3001	3	0	0	1	29.2600	21	0.00799	1.19957	32.7
MO4001	4	0	0	1	31.3748	20	0.00788	1.03444	31.4
MO4010	4	0	1	0	44.5310	20	0.00957	3.22186	31.4

are not significant, we accept model M3001 for the simple reason that it has one less parameter compared to model M4001. Thus the final model is given by (25) and (26) with

$$l' = 0, \quad m' = 1, \quad l = 3 \text{ and } m = 0$$

and the following values for the parameters:

$$\alpha_1 = -0.3337, \quad \alpha_2 = -0.1041, \quad \alpha_3 = -0.3344, \\ b_1 = 0.7826 \quad \text{and} \quad \sigma^2 = 0.0080.$$

The model forecasts for the period $201 \leq i \leq 230$ are plotted in Figure 16.6, along with the historical data for the same period. The match

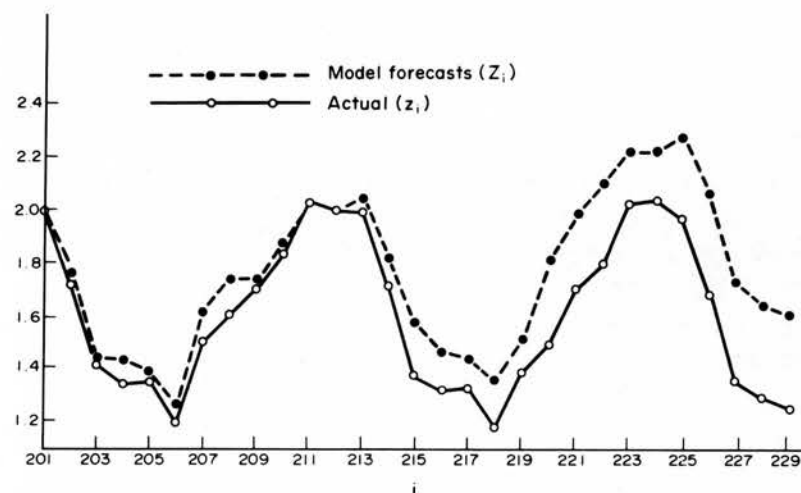


FIGURE 16.6 Validation of Model MO3001.

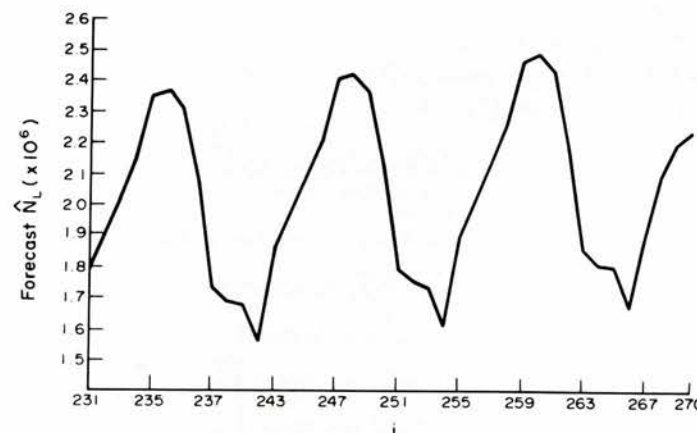


FIGURE 16.7 Forecasts of Model MO3001 until December 1988.

between the two is fairly good. New parameter estimates based on all 230 data points (as opposed to the first 200 data points only) are as follows.

$$\alpha_1 = -0.3263, \quad \alpha_2 = -0.1093, \quad \alpha_3 = -0.3230, \\ b_1 = 0.8008 \quad \text{and} \quad \sigma^2 = 0.0083.$$

Using these estimates the forecasts for the period $231 \leq i \leq 270$ are given in Figure 16.7.

8 Conclusions

In this chapter we have examined a "black-box" approach to modelling, where the modelling is data-dependent. We used an ARMA formulation to model the sequence obtained after removing the linear trend and seasonality in the original data. An alternative approach would have been to model a suitable transformation of the data by an ARMA formulation – e.g. logarithmic transformation of the original data as opposed to the data themselves. Whether such models perform better than the model developed here can only be established by building such models and testing them against that built in this chapter. The main advantage of the model structure used here is that it allows the use of a standard computer package to carry out model building, validation and forecasting.

Notes and References

The historical data used in this case study were obtained from [1].

Further details of the modelling process can be found in any one of the large number of books on time-series modelling; [2]–[6] give a small sample. In particular [2] is a classic, and it discusses the various statistical tests mentioned in this chapter.

We have confined ourselves to linear models; [7]–[9] deal with non-linear models and models with stochastic coefficients.

We used the time series package from [10]; similar packages can be found elsewhere – e.g. [11] and [12].

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PART III
SUPPLEMENTARY MATERIAL

CHAPTER 17

Modelling Exercises

1 Introduction

As mentioned in the Preface, mathematical modelling is best learnt by building models and learning through progressive improvements in the iterative process. This chapter contains a variety of real-world problems for use as exercises in model building.

The problems have been grouped into four categories: biological sciences, physical sciences, social sciences, and engineering and technology. This is done primarily to help the student choose a problem from a discipline of interest.

For each problem we give a brief description and a short list of relevant references. These references contain information to help understand the physical aspects of the problem and a discussion of models built in the past.

An ideal format for carrying out the modelling exercise is as follows:

Step 1: Select a problem of interest.

Step 2: Based on prior knowledge and, if needed, additional information obtained from relevant books (for example, by consulting a subject catalogue in the library) carry out a system characterization and build a mathematical model.

Step 3: Carry out a detailed search using one or more abstracting or indexing journals (for a list of journals, see Chapter 18) to locate models built in the past. For most problems listed in this chapter, a proper search should yield more than one model.

Step 4: Compare critically the model in Step 2 with those from Step 3, considering aspects such as model validity, model complexity, data availability, etc.

Step 5: Revise the model in Step 2 in light of the experience gained in Step 4.

The importance of this sequence is that it forces the student to think deeply about the problem and make an attempt without the thoughts being coloured by the attempts of earlier model builders. However, the earlier models play an essential role as comparators to test ideas and to guide the learning process.

2 Biological Sciences

2.1 Cancer Growth

The development of cancer involves two phases – transformation and growth. In the transformation phase a normal cell changes to an abnormal cell capable of generating a tumour. In the growth phase the abnormal cell multiplies by cell division at a rate higher than that for a normal cell, thus creating tumour growth. In the case of a malignant tumour the growth is so invasive that it can kill the host. The growth of a tumour can be controlled by various means – e.g. radiation or chemotherapy. The problem facing medical researchers is to compare the effectiveness of different policies and to find the most effective policy to control cancer growth. Build a mathematical model to describe growth with and without control action.

References

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2.2 Human Ear

The human ear essentially transforms sound or acoustical signals into electrical impulses for transmission to the brain for processing. Sometimes, due to physiological defects, the ear is incapable of carrying out its normal operations. Often the problem can be rectified through surgical means but in some cases this method does not work. An alternative method for helping such people is through an electromechanical device which in essence is an artificial ear. The problem facing bioengineers is to build an artificial ear whose dynamic behaviour is very similar to that of a normal ear. Build a mathematical model of the dynamics of the human ear to help bioengineers when designing an effective artificial ear.

References

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2.3 Human Joint

Human motion (e.g. walking, lifting, jumping) involves dynamic action at one or more joints in the body. If the joints function normally they cause no discomfort. In many instances a joint does not function normally and causes severe pain when in motion. Typical situations are: joints getting worn with age, the onset of arthritis, joint damage due to an accident, and so on. One way of reducing the pain and discomfort is to replace the defective joint with an artificial one. For the artificial joint to be effective it must be capable of executing all the motions of a normal joint.

Consider a specific joint – e.g. the hip joint. Build a mathematical model to describe the dynamics of the joint so that it is useful to bioengineers when designing hip replacements.

References

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2.4 Renewable Resource

A wide variety of sea life (e.g. fish, crabs, lobsters) are consumed by humans. If the rate of harvesting is higher than the rate of natural increase, the sea life population will decrease and, in the worst case, the species can become extinct. Various international agencies are concerned with this issue and the problem facing them is to decide whether a particular species is to be harvested or not and, if harvesting is to be allowed, what limits should be placed on it. Build a mathematical model which will help the agencies in making sensible decisions.

References

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2.5 Hospital Operation

In most Western countries medical costs are increasing at a very fast rate. There is a strong pressure on hospital administrators to reduce operating costs. Large hospitals provide a variety of medical services to a community. One way of reducing hospital costs is to optimize the allocation of resources (e.g. beds, doctors, nurses) to types of activities (surgical, coronary, pediatrics, etc.) which the hospital must provide. If the allocation is not optimal some of the resources are under-utilized while others are over-strained. In either case the return on investment is not optimal. Build a mathematical model which will help the hospital administrators reduce the cost of operating hospitals.

References

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2.6 Blood Circulation

Proper flow of blood is essential to transmit oxygen and other nutrients to various parts of the body in humans as well as in all other animals. When blood flow is restricted it can cause damage ranging from minor discomfort to death, in the worst case. The flow of blood is influenced by the physiological characteristics of blood vessels – e.g. elastic properties of the wall material, deposition on wall surfaces and so on. These physiological characteristics change with age, eating habits and many other factors. A problem of interest to the medical profession is the relationship between blood flow and physiological characteristics of a blood vessel. Build a mathematical model to characterize this relationship.

References

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2.7 Man–Machine Systems

Many complex machines involve strong interaction between the machine and its human operator; for example, a helicopter and its pilot. For the proper design of such machines the machine and its operator must be viewed as a total system, with due account being given to interaction between the two. As such, models of a human operator are essential in the proper design of machines. For a specific machine, build a mathematical model for a human operator useful in the design of that machine.

References

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2.8 Drug Absorption

Drugs are administered either to fight harmful bacteria responsible for infections or to compensate for imbalances due to some organ malfunction (e.g. insulin in the case of diabetics). A problem facing doctors is deciding the quantity and the frequency of drug administration. If the drug concentration in the human body is too low, the drug is ineffective. On the other hand, if it is too high, it can cause serious side reactions and even death. Build a mathematical model for drug absorption in a human body so that it can be used to determine optimal drug administration policies.

References

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2.9 Genetics

Certain human features (e.g. colour of eye, susceptibility to certain diseases) are inherited genetically. Of particular interest is haemophilia – the case where bleeding does not stop due to a body's inability to produce clotting agents. Both males and females suffer from this disease but it is only the female who is capable of genetically transmitting this defect. In other words, a male suffering

from this defect cannot genetically transmit it to his offspring. Build a mathematical model to predict the spread of this disease in successive generations given the fraction of males and females suffering from it at a particular point of time.

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2.10 Plant Growth

Plants and trees are a renewable source for both humans and animals. We shall confine our attention to trees as a source of woodchips for paper manufacture. When the trees are logged, young seedlings are planted to produce the next generation for harvesting at a later date. The operators of forests and plantations are interested in plants which grow rapidly, so that they can be harvested more frequently. Build a mathematical model to describe plant growth. Such a model is of use in devising optimal harvesting policies to maximize woodchip yield.

References

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3 Engineering and Technology

3.1 Internal Combustion Engine

The power source in a gasoline driven car is an internal combustion engine (ICE) which converts the chemical energy of gasoline into mechanical energy by the process of combustion. The efficiency of the engine and the pollution generated depends critically on the combustion process. The design of an efficient engine requires a good understanding of the combustion process inside the ICE. Build a mathematical model of the combustion process so that it is of use to design engineers when designing better engines.

References

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3.2 Traffic Flow

Traffic flow in the heart of a big city depends critically on the traffic control scheme. The scheme comprises: (i) the traffic light cycle at each intersection, and (ii) the synchronization between traffic lights at different intersections. The traffic light cycle consists of a sequence of red, amber and green signals of either fixed or variable duration. If the control scheme is poor, long lines can result at one or more of the intersections increasing the time to travel across the city. The problem facing the traffic engineer is to evolve a scheme which minimizes the expected time to travel across the city. Build a mathematical model to solve this problem.

References

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3.3 Technology Substitution

One of the characteristics of modern industrial societies is that old products are constantly being replaced by new ones. There are various reasons for this – products having a finite lifetime, technological changes causing the old product to become obsolete, etc. The process of an old product (e.g. black and white television) being replaced by a new product (e.g. colour television) over time is called “technology substitution”.

Technology substitution is important to the manufacturers of new products when planning production to meet the expected demand. Build a mathematical model which can be used to forecast technology substitution.

References

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3.4 Power System Dynamics

A power system is a collection of a number of power-generating units connected as a network to supply demand at different points in the network. Whenever a sudden change occurs (e.g. due to a short-circuit) the stability of the system is affected. If proper action is not initiated within a reasonable time the system can fail catastrophically, resulting in major blackouts. A problem of interest to power engineers is the dynamic behaviour of the system for different types of faults (or sudden changes) under different control actions. Build a mathematical model to help the engineer study the problem.

References

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3.5 Research and Development Management

Research and development (R&D) is an important activity in any modern industrial organization. The long-term viability of the organization depends on successful R&D activities. The R&D manager is faced with the difficult problem of allocating limited resources (money, manpower, space, etc.) between a number of competing projects. Since project outcome (i.e. success or failure) and potential commercial gain should the project be a success are uncertain, the problem of allocation becomes more difficult. Build a mathematical model which will help the R&D manager to make right decisions.

References

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- [4] Kamien, M. I. and Schwartz, N. L.: *Market Structure and Innovation*. Cambridge University Press, Cambridge, 1982.

3.6 Product Warranty

Warranty is a contractual obligation which requires the manufacturer to either repair or replace a product free of cost should the product fail within a pre-specified period (called the warranty period) subsequent to a sale. Warranty is sometimes imposed on the manufacturer to protect consumer interests, but often manufacturers offer it as a means to advertise product quality. Warranty servicing costs money and hence affects profitability. Manufacturers would like to have estimates of this cost as a function of warranty period before they make decisions on the warranty to be offered. Build a mathematical model which will help solve this problem.

References

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3.7 Quality Control

In multi-stage production systems the product quality at the output of the final stage is a function of the input materials and the condition of the machines. Poor quality affects sales and hence the revenue generated. Quality can be controlled by proper inspection of the product during the intermediate stages of its production and by effective maintenance of the machines. These cost money. Hence, a sensible scheme must be employed to maximize the total profits. Build a mathematical model which will yield the optimal inspection and maintenance policies to maximize the total profits.

References

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3.8 Process Control

In a chemical process the output quality and yield depends critically on the levels assigned to relevant factors (temperature, pressure, concentration, etc.).

It is important to optimally select these levels as well as to monitor and control the system to ensure that they stay at the desired levels. Build a mathematical model to help achieve this.

References

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3.9 Software Reliability

Software reliability is important to computer manufacturers as well as users. The lack of reliability arises due to hidden faults (also called “bugs”) which affect computer performance. The reliability is improved through testing to detect faults and by rectification of the detected faults. This is a costly process in terms of time and money. Build a mathematical model to describe the occurrence of faults and their discovery. Such a model is of use in making decisions with respect to the effort to be spent in testing.

References

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3.10 Image Modelling

Biomedical images are used to detect medical disorders and problems. In the past the images were processed by doctors through visual examination. With the rapid developments in digital computers there is a trend towards the use of computers for image processing and diagnosis. For the computer to diagnose correctly with high reliability requires correct image models. Build a mathematical model for processing X-ray images to detect a specific medical problem.

References

- [1] Sklansky, J. and Bisconte, J. C. (eds): *Bio-Medical Images and Computers*. Springer-Verlag, Berlin, 1982.

- [2] Preston, K. and Uhr, L. (eds): *Multicomputers and Image Processing: Algorithms and Programs*. Academic Press, New York, 1982.
- [3] Rosenfeld, A. (ed.): *Image Modelling*. Academic Press, New York, 1981.
- [4] Jain, A. K.: Advances in mathematical models for image processing, *Proc. IEEE*, 69 (1981), 502–28.

4 Physical Sciences

4.1 Ocean Waves

Exploration of natural resources under the ocean floor requires use of offshore structures such as platforms. These structures are subjected to constant beating by ocean waves. Hence the design of such structures requires the modelling of the dynamic loading effects of wave action. Build a mathematical model to describe the wave action on fixed structures so that it can be used in the proper design of offshore structures.

References

- [1] LeBlond, P. H. and Mysak, L. A.: *Waves in the Ocean*. Elsevier, Amsterdam, 1978.
- [2] Kinsman, B.: *Wind Waves: Their Generation and Propagation on the Ocean Surface*. Prentice-Hall, Englewood Cliffs, NJ, 1965.
- [3] LeBlond, P. H. and Mysak, L. A.: Ocean waves: a survey of some recent results, *SIAM Rev.*, 21 (1979), 289–328.
- [4] Meyers, R. E.: *Waves on Beaches and Resulting Sediment Transport*. Academic Press, New York, 1972.

4.2 Sand Dunes

The formation of sand dunes and their encroachment into de-forested lands near deserts has become a serious problem in many parts of the world. The problem of interest is the movement of sand dunes. A model is needed to predict the spread of desert, as well as to devise policies to control the spread. Build a mathematical model to describe the movement of sand dunes.

References

- [1] Bagnold, R. A.: *The Physics of Blown Sand and Desert Dunes*. Methuen, London, 1954.
- [2] Yalin, M. S.: *Mechanics of Sediment Transport*, 2nd edn. Pergamon Press, Oxford, 1977.
- [3] Brown, R. A.: *Analytical Methods in Planetary Boundary-layer Modelling*. Halsted Press/Wiley, New York, 1974.
- [4] Cekirge, H. M. et al.: Movements of sand dunes: I. Two-dimensional model, *Math. Modelling*, 3 (1982), 371–84.

4.3 Water Seepage

Dams are built across rivers to store water for multiple uses – irrigation, power generation, flood control, etc. Some of the water stored is lost due to

evaporation and seepage through the ground. Before a dam is to be built, it is important to estimate these losses. If the losses are significant, then the viability of the dam is in question. To obtain an estimate of seepage loss one must develop a theory for seepage. Build a mathematical model to describe the theory of water seepage through porous media.

References

- [1] Rushton, K. R. and Redshaw, S. C.: *Seepage and Groundwater Flow: Numerical Analysis by Analog and Digital Methods*. Wiley, Chichester, 1979.
- [2] Verruijt, A.: *Theory of Ground-Water Flow*. Macmillan, New York, 1970.
- [3] Lloyd, E. H. et al. (eds): *The Mathematics of Hydrology and Water Resources*. Academic Press, New York, 1979.
- [4] Bear, J.: *Dynamics of Fluids in Porous Media*. Elsevier, New York, 1972.

4.4 Atmospheric Pollution

Most industrial processes emit various chemicals into the atmosphere. These get transmitted over large distances and often affect the ecology when they return to ground in the form of acid rain or other undesirable fallout. As such, many regulating authorities require an ecological evaluation of the potential damage that can be caused under the worst scenario before permission is granted to build large industrial plants. Build a mathematical model which will predict the dispersion of pollutants in the atmosphere and so be useful in evaluating potential ecological damage.

References

- [1] Crank, J.: *The Mathematics of Diffusion*. Clarendon Press, Oxford, 1956.
- [2] Weber, E. (ed.): *Air Pollution: Assessment Methodology and Modelling*. Plenum Press, New York, 1982.
- [3] Brebbia, C. A. (ed.): *Mathematical Models for Environmental Problems*. Pentech Press, London, 1976.
- [4] Hidy, G. M. and Brock, J.: *The Dynamics of Aero-Colloidal Systems*. Pergamon Press, Oxford, 1971.

4.5 Forest Fires

A forest fire occurs when dry vegetation in a forest burns in an uncontrolled manner. It is a natural phenomenon initiated by a lightning strike or some other ignition event. The burning and spread of forest fires is a complicated phenomenon, an understanding of which will help in fighting such fires should they occur close to human settlements. Build a mathematical model to describe the burning and the spread of forest fires.

References

- [1] Strehlow, R. A.: *Combustion Fundamentals*. McGraw-Hill, New York, 1984.
- [2] Kanury, A. M.: *Introduction to Combustion Phenomena (for fire, incineration, pollution and energy applications)*. Gordon & Breach, New York, 1975.

- [3] Spalding, D. B.: Mathematical models of turbulent flames: a review, *Comb. Sci. Tech.*, **13** (1976), 3-25.
- [4] Zel'dovich, Ya. B. et al.: *The Mathematical Theory of Combustion and Explosions*. Consultants Bureau, New York, 1985.

4.6 Oil Spillage

Oil spillage in rivers and oceans is a matter of concern to environmental authorities as it can lead to serious ecological damage as well as severe economic losses. A model which can predict the movements of a patch of oil is of use to authorities to plan strategies to minimize the damage caused by the spill. Build a mathematical model which can predict the movement of an oil spill in a large bay.

References

- [1] Nihoul, J. C. (ed.): *Modelling of Marine Systems*. Elsevier, New York, 1975.
- [2] Ippen, A. T. (ed.): *Estuary and Coastline Hydro Dynamics*. McGraw-Hill, New York, 1966.
- [3] Nelson-Smith, A.: *Oil Pollution and Marine Ecology*. Plenum Press, New York, 1973.
- [4] Wardley-Smith, J. (ed.): *The Control of Oil Pollution on the Sea and Inland Waters*. Graham & Trotman, London, 1976.

4.7 Oil Extraction

The efficient extraction of oil from underground reservoirs is of great importance due to the ever-increasing demand for oil. In order to develop efficient methods, one needs a model of the behaviour of hydrocarbon reservoirs. Build a mathematical model which will help solve the problem.

References

- [1] Shah, D. O. and Schechter, R. S. (eds): *Improved Oil Recovery by Surfactant and Polymer Flooding*. Academic Press, New York, 1977.
- [2] Aziz, K. and Settari, A.: *Petroleum Reservoir Simulation*. Applied Science Publishers, London, 1979.
- [3] Odeh, A. S.: An overview of mathematical modeling of the behaviour of hydrocarbon reservoirs, *SIAM Rev.*, **24** (1982), 263-73.
- [4] Owen, D. B. (ed.): *The Search for Oil: Some Statistical Methods and Techniques*. Marcel Dekker, New York, 1975.

4.8 Waste Water Treatment

In disposing of waste water it is important to ensure that it does not affect the water supply system. This is done by treating the waste water either using chemicals or by some natural process. Build a mathematical model to describe the underlying processes involved in waste water treatment. Such a model is of use in devising economical and effective treatment policies for waste water.

References

- [1] Canale, R. P. (ed.): *Biological Waste Treatment*. Wiley-Interscience, New York, 1971.
- [2] Morley, D. A.: *Mathematical Modelling in Water and Wastewater Treatment*. Intel Ideas, Philadelphia, PA, 1979.
- [3] Lam, D. C. L. et al. (eds): *Effluent Transport and Diffusion Models for the Coastal Zone*. Springer-Verlag, New York, 1984.
- [4] Deininger, R. A. (ed.): *Models for Environmental Pollution Control*. Ann Arbor Scientific, Ann Arbor, MI, 1973.

4.9 Semiconductor Devices

Semiconductor devices are used extensively in many applications. The analysis of electronic circuits involving such devices requires appropriate mathematical models of the devices. Build a mathematical model to describe the dynamic behaviour of semiconductor devices of a particular type.

References

- [1] Sze, S. M.: *Physics of Semiconductor Devices*, 2nd edn. Wiley, New York, 1981.
- [2] Wang, Y. C.: Review of some mathematical models of non-linear domain dynamics in bulk effect semiconductors, *J. IMA*, **11** (1973), 251–80.
- [3] Bank, R. E. et al.: Numerical methods for semiconductor device simulation, *SIAM J. Stat. Sci. Comp.*, **4** (1983), 416–35.
- [4] Cox, W.: Mathematical modelling in microphysical technology, *Int. J. Math. Educ. Sci. Technol.*, **17** (1986), 1–24.

4.10 Fatigue Failure

A fairly common cause for mechanical component failure is the onset and growth of a fatigue crack. The time to component failure (or equivalently, the lifetime of the component) depends on various factors, the important one being the mechanical loading history. A relationship between the time to failure with the relevant factors is useful in the design and operation of the components. Build a mathematical model which can be used to predict fatigue failure in components.

References

- [1] Chang, J. B. and Hudson, C. M. (eds): *Methods and Models for Predicting Fatigue Crack Growth Under Random Loading*. American Society for Testing Materials, Philadelphia, PA, 1981.
- [2] Little, R. E. and Ekvall, J. C. (eds): *Statistical Analysis of Fatigue Data*. American Society for Testing Materials, Philadelphia, PA, 1981.
- [3] Little, R. E. and Jebe, E. H. (eds): *Statistical Design of Fatigue Experiments*. Wiley, New York, 1975.
- [4] Heller, R. A. (ed.): *Probabilistic Aspects of Fatigue*. American Society for Testing Materials, Philadelphia, PA, 1971.

5 Social Sciences

5.1 Advertising

Advertising is a means by which a manufacturer can promote the product and improve sales and, hence, the revenue generated. However, advertising costs money and is worthwhile only if the cost of advertising is less than the increase in the sales revenue. The problem facing the manufacturer is to evaluate the effectiveness of different advertising policies and the selection of the optimal policy. Build a mathematical model to help solve this problem.

References

- [1] Schmalensee, R.: *The Economics of Advertising*. North-Holland, Amsterdam, 1972.
- [2] Gensch, D. H.: *Advertising Planning: Mathematical Models in Advertising Media Planning*. Elsevier, Amsterdam, 1973.
- [3] Little, J. D. C.: Aggregate advertising models: a state of the art, *Oper. Res.*, **27** (1979), 629–67.
- [4] Sethi, S. P.: Dynamic optimal control models in advertising: a survey, *SIAM Rev.*, **19** (1977), 685–725.

5.2 Perishable Item Inventory

Retailers of perishable items (e.g. milk, fruits, vegetables) face a dilemma. If they have a large inventory, they might be forced to discard items not sold within a time period determined by the shelf-life of the item. This causes economic loss. On the other hand, if the inventory is low, they face the prospect of reduced profit due to unsatisfied customers. The problem is made complicated by variable ordering costs and uncertainty in demand. Build a mathematical model to obtain optimal ordering policies and inventory levels to maximize the expected profit.

References

- [1] Tersine, R. J.: *Principles of Inventory and Materials Management*, 2nd edn. North Holland, Amsterdam, 1982.
- [2] Nahmias, S.: Perishable inventory theory: a review, *Oper. Res.*, **30** (1982), 680–708.
- [3] Tinarelli, G. U.: Inventory control: models and problems, *Eur. J. Oper. Res.*, **14** (1983), 1–12.
- [4] Silver, E. A.: Operations research in inventory management: a review and critique, *Oper. Res.*, **29** (1981), 628–45.

5.3 Insurance Premiums

The economic viability of an insurance company depends critically on its ability to assess risks and decide on the premium charged to cover risks. If the premiums are low, then payouts can exceed revenue collected and the company can go bankrupt. On the other hand, if they are high, the number of customers will go down, thus affecting profitability. The problem facing an

insurance company is the premium it should charge for different risks to ensure economic viability and maximize its profits.

References

- [1] Beard, R. E. et al.: *Risk Theory – The Stochastic Basis of Insurance*, 3rd edn. Chapman & Hall, London, 1984.
- [2] Buhlmann, H.: *Mathematical Methods in Risk Theory*. Springer-Verlag, New York, 1970.
- [3] Moore, P. G.: *The Business of Risk*. Cambridge University Press, London, 1983.

5.4 Supermarket Location

A retailer is planning to open a chain of new supermarkets in a big metropolitan area. The problem facing the retailer is deciding on the number and the location for the supermarkets. Wrong locations, and too few or too many, will affect the profitability of the venture. Build a mathematical model which will assist the retailer in making the right decision.

References

- [1] Masser, I.: *Analytical Models for Urban and Regional Planning*. David & Charles, North Pomfret, VT, 1972.
- [2] Wilson, A. G. and Kirkby, M. J.: *Mathematical Methods for Geographers and Planners*. Oxford University Press, Oxford, 1975.
- [3] Helly, W.: *Urban System Models*. Academic Press, New York, 1975.
- [4] Larson, R. C. and Odoni, A. R.: *Urban Operations Research*. Prentice-Hall, Englewood Cliffs, NJ, 1981.

5.5 Oil Exploration

An oil exploration company has to make a decision on the location of the next hole to be drilled. If the drilled hole turns out to be dry then the investment (cost of drilling) is a total loss. If the hole yields gas it is a partial success, and if the outcome is oil it is a total success. The company owns leases at many different locations. The decision problem is made difficult because of the uncertainty in the outcome, as well as due to the fact that only imperfect information can be obtained by doing some testing. Build a mathematical model which will help the company in making the right decision to maximize its expected profits.

References

- [1] Finlay, P. N.: *Mathematical Modelling in Business Decision Making*. St Martin's Press, London, 1985.
- [2] Baird, B. F.: *Introduction to Decision Analysis*. Duxbury Press, Mass., 1978.
- [3] Rivett, P.: *Model Building for Decision Analysis*. Wiley, Chichester, 1980.
- [4] Holloway, C. A.: *Decision Making Under Uncertainty: Models and Choices*. Prentice-Hall, Englewood Cliffs, NJ, 1979.

5.6 National Economy

The state of a national economy is defined through aggregate variables such as GNP, interest rates, inflation, trade balance, unemployment, etc. These variables interact in a dynamic way. Thus an action to influence one variable can lead to undesirable changes in one or more of the remaining variables. As a result models which can predict the consequences of different actions would be of immense help both to economists and politicians. Build a mathematical model which will predict the effect of different control actions.

References

- [1] Kogiku, K.: *An Introduction to Macro-Economic Models*. McGraw-Hill, New York, 1968.
- [2] Cuthbertson, K.: *Macroeconomic Policy*. Macmillan, New York, 1979.
- [3] Allen, R. G. D.: *Macro-Economic Theory: A Mathematical Treatment*. Macmillan, New York, 1967.
- [4] Shapiro, E. (ed.): *Macroeconomics: Selected Readings*. Harcourt, Brace & World Inc., New York, 1970.

5.7 Brand Switching

A shopkeeper stocks a wide variety of cigarette brands and is constantly faced with the problem of running short of certain brands and being left with large inventories of other brands due to customers changing their choice of brands. As a consequence, the profits of the shopkeeper are reduced. Build a mathematical model which will help the shopkeeper optimize on his ordering policies, taking into account the random nature of brand switching.

References

- [1] Massy, W. F. et al.: *Stochastic Models of Buying Behavior*. MIT Press, Cambridge, MA, 1970.
- [2] Kollat, D. T. et al. (eds): *Research in Consumer Behavior*. Holt, Rinehart & Winston, New York, 1970.
- [3] Devletoglou, N.: *Consumer Behavior: An Experiment in Analytical Economics*. Harper & Row, New York, 1971.
- [4] Weddepohl, H. N.: *Axiomatic Choice Models and Duality*. Rotterdam University Press, Rotterdam, 1970.

5.8 Learning Behaviour

One way in which young children can be encouraged to learn is by a process of reward when there is positive response, and no reward (or sometimes punishment) with negative response. A problem of interest to educators is to devise schemes that will improve the rate of learning. Build a mathematical model which can be used to evaluate different schemes before they are tried on the children.

References

- [1] Norman, M. F.: *Markov Processes and Learning Models*. Academic Press, New York, 1972.
- [2] Yelle, L. E.: The learning curve: historical review and comprehensive survey. *Dec. Sci.*, **10** (1979), 302–28.
- [3] Herkenrath, U. et al. (eds): *Mathematical Learning Models: Thoery and Algorithms*. Springer-Verlag, New York, 1983.
- [4] Atkinson, R. C. et al.: *An Introduction to Mathematical Learning Theory*. Wiley, New York, 1965.

5.9 Resource Depletion

One of the serious problems facing mankind is that, with the increasing population and the rate of consumption, there is a possibility of running out of various natural resources in a fairly short time interval. Economic planners need estimates for the time intervals for the exhaustion of different resources under various policies for consumption. This information is also useful in initiating conservation schemes and initiating research into alternatives. Build a mathematical model which will yield the desired answers.

References

- [1] Meadows, D. L. and Singer, S. F.: *The Limits to Growth: A Debate*. American Association for the Advancement of Science, Washington, DC, 1973.
- [2] Churchman, C. W. and Mason, R. O. (eds): *World Modelling: A Dialogue*. Elsevier, New York, 1976.
- [3] Dayal, R.: *An Integrated System of World Models*. North Holland, Amsterdam, 1981.
- [4] Marois, M. (ed.): *Design of Global System Models and Their Limitations*. Pergamon Press, Oxford, 1977.

5.10 Population Migration

In all countries there is a constant migration of people from one region to another. The reasons for such migration are many. A problem of interest to planners is the prediction of population migration. Build a mathematical model to obtain predictions of population migration.

References

- [1] Rees, P. H. and Wilson, A. G.: *Spatial Population Analysis*. Arnold, London, 1977.
- [2] Cebula, R. J.: *The Determinants of Human Migration*. Lexington Books, Lexington, MA, 1979.
- [3] Rogers, A.: *Introduction to Multi-Regional Mathematical Demography*. Wiley, New York, 1975.
- [4] Lowry, I. S.: *Migration and Metropolitan Growth: Two Analytical Models*. Chandler, San Francisco, CA, 1966.

CHAPTER 18

Reference Material

1 Introduction

As indicated in the Preface, the list of books on mathematical models and modelling is large. In Section 2 we give a comprehensive list of such books, along with a comparative evaluation and annotation so that they can be used as sources for additional material to supplement the text. In Section 3 we give a list of journal articles on models, modelling and teaching modelling, primarily for the instructor's use. The articles are arranged alphabetically by author. We conclude by giving a list of abstracting journals on mathematical modelling, which the student will find useful when model building.

2 Books on Models and Modelling*

2.1 Framework for Comparative Evaluation

As seen from Part I, mathematical modelling requires an understanding of many different topics. Effective teaching of mathematical modelling requires that the student be exposed to all of these topics. Broadly speaking the different topics needed for modelling closely follow the chapters in this book and are as follows:

- A. Models and model building
- B. System characterization
- C. Different mathematical formulations
- D. Analysis of mathematical formulations
- E. Parameter estimation
- F. Design of experiment
- G. Validation

*This section is based on: A comparative evaluation of books on mathematical modelling, *Math. Modelling*, **9** (1987), 17–28.

For the purpose of comparative evaluation, we divide topics C and D into further subtopics as follows:

- C1. Static formulations (deterministic/probabilistic)
- C2. Dynamic deterministic formulations
- C3. Dynamic stochastic formulations

and

- D1. Analytical methods
- D2. Computational methods
- D3. Simulation methods

(Many of these can be further subdivided, e.g. C2 can be subdivided into difference equations, ordinary differential equations, partial differential equations and so on, but the subdivision shown above is sufficient for the review process.)

We include a further topic to show the totality of the modelling process.

H. Application/Case studies

and this is subdivided into four subtopics as follows:

- H1. Physical sciences
- H2. Biological sciences
- H3. Social sciences
- H4. Technology

As a result we have a total of sixteen topics/subtopics, and these form the basis for the comparative evaluation.

2.2 Comparative Evaluation

Table 18.1 gives the topics/subtopics covered by each of the books included for evaluation. This is indicated by an x in the appropriate column. A few comments are appropriate at this stage:

- (i) If a book concentrates on one method of analysis we classify the book as covering that particular method of analysis and ignoring other methods.
- (ii) If a book concentrates on some types of formulations more than others, then it is classified as examining only those types covered in greater detail.
- (iii) For topics, E, F and G we use the following convention: a book covers a topic if either a chapter is devoted to it or if the topic is stressed

TABLE 18.1 Comparative Evaluation of Books on Mathematical Modelling

Authors	A	B	C1	C2	C3	D1	D2	D3	E	F	G	H1	H2	H3	H4
Ahuja and Schachter	x	x	x	x		x	x	x		x	x	x	x	x	x
Andrews and McLone	x	x	x	x	x	x						x	x	x	x
Aris	x	x	x	x	x	x									x
Avula <i>et al.</i>	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Bender	x	x	x	x		x		x							
Boyce		x	x	x	x	x						x	x		x
Boynton	x		x			x								x	
Bradley <i>et al.</i>		x	x	x		x	x					x			x
Brams <i>et al.</i>	x	x	x			x						x	x		x
Braun <i>et al.</i>	x	x		x		x						x	x		x
Burghes and Wood	x	x	x	x		x								x	
Burghes <i>et al.</i>	x	x	x	x	x	x						x	x	x	x
Clark	x	x	x	x		x	x			x			x		x
Close and Frederick	x	x		x		x						x		x	
Coats and Parkins	x	x		x				x					x	x	
Dym and Ivey	x	x	x	x		x						x	x	x	x
Giordano and Weir	x	x	x	x		x	x	x	x	x		x	x	x	x
Greenspan		x		x			x					x			
Haberman	x	x		x		x						x	x		x
Hawkes		x												x	
Howard	x	x		x								x			x
Hyvarinen	x	x	x							x					x
James	x	x	x	x		x	x					x	x		x
James and McDonald	x	x	x	x		x		x					x	x	x
Kemeny and Snell	x	x	x	x	x	x								x	
Lancaster	x	x	x	x		x						x	x		
Lucas <i>et al.</i>	x	x	x			x		x						x	x
Maki and Thompson	x	x	x	x	x	x		x					x	x	
Malkewitch and Meyer	x	x	x	x	x	x	x			x	x			x	
Marchuk and Nisevich	x	x	x	x		x	x						x		
Marcus <i>et al.</i>		x			x	x							x		
McClamroch	x	x		x		x		x							x
Mihram	x		x		x			x							
Nicholson		x	x	x		x	x	x							x
Noble	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Olinick	x	x	x	x	x	x							x	x	
Osborne and Watts	x	x			x			x			x		x	x	x
Ransom	x	x	x	x	x	x	x	x					x		
Rivett	x	x	x			x		x						x	
Roberts	x	x	x			x							x	x	
Ross					x	x			x						
Saaty	x	x	x	x	x	x	x	x	x			x	x	x	
Saaty and Alexander	x	x	x	x	x	x						x	x	x	
Smith	x	x	x		x			x							x
Spriet <i>et al.</i>	x	x		x	x	x	x	x	x				x		x
Weinberg	x	x	x	x	x							x	x	x	x
Zeigler	x	x			x			x					x		
Ziercp		x		x		x						x			

significantly throughout the book so that it is treated as being of importance in the modelling process.

- (iv) For topic H (subtopics H1–H4) the basis for classification is again the relative importance given to applications/case studies from each of the four disciplines.

Brief descriptive comments are given on each book.

Ahuja and Schachter (1983) This book presents formal models of spatial patterns. Examining the sequence of steps involved in modelling beginning with model conception analysis, fitting, and ending with synthesis of data, the book illustrates the various phases of modelling and synthesis.

Andrews and McLone (1976) This is a collection of modelling exercises written by different authors. Seven of the exercises are from either physical sciences or technology; two from biological sciences and five from social sciences. In addition there is a chapter each on network flow models and role of the catastrophe method. The main emphasis is on model formulation.

Aris (1978) This book concentrates mainly on the use of ordinary differential equation formulations (lumped models) and partial differential equation formulations (distributed models) in modelling systems and processes in chemical engineering. The emphasis is on modelling and analytical methods of analysis. The appendices examine three case studies.

Avula, Kalman, Liapis, and Rodin (1984) This is a volume of papers presented at the Fourth International Conference on Mathematical Modelling. It contains seven invited lectures concerning topics such as deterministic control, multicriterion decision making, and the use of iterative graphics. Other subjects covered extensively include methodology, systems theory, parameter estimation and system identification, optimization, stochastic modelling in economics, transportation, and mathematical modelling education.

Bender (1978) This is a rather unusual book. It is divided into two parts. Part I deals mainly with models involving non-dynamic formulations. The chapter entitled "Arguments from Scale" is interesting. Part II deals with models involving simple ordinary differential equation formulations. The model building and analysis are strongly interwoven and the range of applications considered is large and varied.

Berry et al. (eds) (1986) This is a collection of 23 articles dealing with various issues related to mathematical modelling; the teaching of mathematical modelling and a variety of case studies with a particular emphasis on the role and use of microcomputers.

Berry et al. (eds) (1987) This is a collection of 25 articles grouped under two headings: (A) Modelling Courses and (B) Modelling and Schools. The articles discuss various issues related to the teaching of mathematical modelling at different levels and in different disciplines.

Boyce (ed.) (1981) This is a collection of seven case studies written by different authors. The topics covered are herbicide resistance, elevator system, traffic flow, semiconductor crystal growth, railroad/information (network flow models), computer data communication and system security verification. The case study on semiconductor crystal growth (by L. O. Wilson) is especially interesting, for it describes the evolution of the modelling process very nicely.

Boynton (1980) This is an introductory book that combines the logic of mathematics with the art of politics. It assumes a knowledge of algebra to study discrete time systems. Applications of the book include such special issues as policy outputs, voting distributions and behaviour regulation.

Bradley, Gibson and Cross (1981) This is a collection of seven case studies to model systems of processes from different industries and written by different authors. The topics covered are: blast furnaces, sound distribution in a record player, hydraulic buffers, grinding of particles, moving fresh glass, motion of an automobile, and freezing and thawing of meat. Each case study is a result of group activity and often the group leader presents his modelling attempt and compares it with that of the group.

Brams, Lucas and Straffin (eds) (1983) This book is a collection of 13 case studies written by different people. Each case study deals with the modelling and analysis of a topic from a political or related field. In some cases the model analysis is compared with the real data. Each case study ends with notes for the instructor.

Braun, Coleman and Drew (eds) (1982) This book deals exclusively with models involving differential equation formulations. It consists of 23 chapters divided into five parts: Part 1 is general; Part 2 deals with modelling exercises involving first-order differential equation formulations; Part 3 (4) deals with three (four) modelling exercises involving higher-order linear differential equation (partial differential equation) formulations; Part 5 deals with modelling different facets of traffic flow, and Part 6 deals similarly with population interactions.

Burghes and Wood (1979) This book deals mainly with very simple mathematical formulations; their analysis and application to problems in social science. The emphasis is on deterministic non-dynamic formulations, with a chapter each on difference and first- and second-order differential equations.

Burghes, Huntley and McDonald (1982) The book consists of four parts: Part 1 deals with interesting case studies; Part 2 is a collection of 20 simple modelling exercises involving mainly deterministic formulations (either non-dynamic or simple ordinary differential equation formulations), in some cases real data is used for modelling and validation; Part 3 deals with the modelling process in a formal sense; and the last part contains 20 topics suitable for student modelling assignments.

Clark (1976) This book discusses mathematical models applicable to the optimal utilization of biological resources focusing on conservation of productive resources rather than the preservation of natural environments. A general model is put forth and then in succeeding chapters mathematical techniques of optimal control theory and dynamical systems are introduced.

Close and Frederick (1978) This book provides exposure to dynamic systems. Assuming a knowledge of differential and integral calculus the authors cover mechanical, electrical, electromechanical, thermal, and hydraulic systems. They also include five case studies drawn from a variety of systems, including a sociological system, a thermal system, and a velocity control system.

Coats and Parkin (1977) This book concentrates on computer modelling for social sciences. The first five chapters deal with models and modelling. The last three chapters deal with three case studies. The topics for the case studies are: human memory; bed usage in hospitals; and economics of education.

Dym and Ivey (1980) This book is unusual in its presentation. It consists of two parts: Part A deals with what the authors call "mathematical ideas of interest to the model builder" and contains four chapters. The chapters on dimensional analysis and on scaling are particularly interesting. Part B deals with applications and contains 10 chapters. A chapter each is devoted to ordinary differential equation formulation models and linear programming models. Two chapters deal with oscillations and there are chapters on traffic flow and diffraction.

Giordano and Weir (1985) This book places emphasis on identifying problems and their underlying assumptions, determining appropriate data to be collected, constructing and selecting models, and testing and validating models. It provides numerous examples and applications in mathematical sciences, operations research, engineering, social and life sciences, and management science.

Greenspan (1973) This book concentrates on the use of difference equation formulations to model a range of problems in dynamics and fluid mechanics. The emphasis is solely on the model building.

Haberman (1977) This book examines modelling in three areas – mechanical vibrations, population growth, and traffic flow. In each area a series of models are developed with a lot of emphasis on the analysis and interpretation of the model. The book is unusual in the sense that system understanding, modelling and analysis are strongly interwoven.

Hawkes (ed.) (1973) This is a collection of articles dealing with trends in mathematical modelling in mainly social sciences.

Howard (1979) This book deals with partial differential equation formulation in modelling problems in particle dynamics, fluid mechanics, cosmology, and application of models in aeronautical engineering.

Hyvarinen (1970) This book deals mainly with the use of non-dynamic formulations (especially regression formulations) in modelling industrial processes. It contains a chapter on design of experiments and two chapters on the analysis of experimental results.

James (1978) This book is a revised version of the *Proceedings of the Conference on the Use of Mathematical Modeling in Water Pollution Control*. Nineteen papers are included. Techniques of water pollution control systems are developed, as are models that apply to polluted environments, waste treatment and water resources.

James and McDonald (1981) This book contains 15 case studies written by different authors. They cover a wide range of topics and the emphasis is mostly on model building. One or two case studies involve simulation. The models involve mainly non-dynamic formulations and the dynamic models discussed are based on simple ordinary differential equation formulations.

Kemeny and Snell (1972) This is a reprint of an old book first published in 1962. It deals with seven case studies from social sciences and one from biological science. The topics covered include: ecology, money flow, organization, scheduling, and a few others. The modelling involves both deterministic and stochastic formulations.

Lancaster (1976) This book contains chapters on growth of populations, on population genetics, and on collision of particles. In particular, the last modelling exercise discusses models under different assumptions and laws. In addition there are chapters on linear programming and on search for maximum.

Lucas, Roberts and Thrall (eds) (1983) This book contains a large number of modelling exercises dealing with application to economics, traffic theory, operations research and other fields. The models involve mainly non-dynamic

formulations. A few of the exercises involve computer simulation but the majority use analytical methods of analysis. The range of topics covered is fairly wide. There are two interesting case studies involving problems in power engineering.

Maki and Thompson (1973) This book takes an axiomatic approach to model building. It discusses modelling topics from biological and social sciences involving both deterministic and stochastic dynamic model formulations. The last chapter, entitled "Practical aspects of model building", discusses intuitive evaluation, statistics for the model building process and simulation.

Marchuk and Nisevich (1980) This book concerns the application of mathematical theory to medicine. In particular it introduces a mathematical model of viral disease and then develops methods for quantitative assessment of the seriousness of viral hepatitis. These models are then used to study the dynamics of functional recovery.

Marcus-Roberts and Thompson (eds) (1983) This book is a collection of 12 case studies in biological sciences written by different authors. The case studies involve both deterministic and stochastic dynamic formulations and in some of the studies real data are used. The emphasis is on models suitable for analytical methods of analysis. Each chapter contains notes at the end for the instructor.

McClamroch (1980) This book concentrates on models involving mainly ordinary differential equation formulations. Seven chapters are devoted to differential equation models. In each chapter several interesting case studies/applications are discussed. Both modelling and analysis are equally emphasized. Most of the case studies come from engineering, and an appendix deals with CSMP simulation.

Mihram (1972) This book concentrates mainly on probabilistic non-dynamic and discrete stochastic process formulations. The emphasis is on computer simulation. In addition, it contains two chapters on the design of experiment.

Nicholson - Vol. 2 (1980) This book is a collection of seven case studies from various branches of engineering. The topics for the case studies are: iron and steel making, electric arc furnace, turbo generator, mineral extraction, and manufacturing. The models involve either non-dynamic or simple differential equation formulations.

Noble (1967) This book is based on examples of applications of undergradu-

ate mathematics in engineering, submitted by various university mathematics and engineering departments and some industrial companies. The four sections of the book deal with applications of elementary mathematics, ordinary differential equations, field problems such as flow of fluids or heat, the diffusion of gases, stresses and strains in solids, linear algebra, and probability.

Olinick (1978) This book contains 14 chapters, with 10 devoted to modelling specific topics. In each modelling chapter often more than one model is built and analysed. The interesting aspect is the historical perspective for modelling topic. The models are mainly from biological and social sciences and involve a range of mathematical formulations.

Osborne and Watts (eds) (1977) This is a collection of several articles with the emphasis on simulation. Six of them deal with case studies from mainly biological and social sciences. One chapter deals with the use of statistics in model validation.

Ransom (1981) This book describes the uses and applications of models in development biology. A variety of model systems are discussed in the first half of the book. The second half concentrates on computer modelling.

Rivett (1972) This book contains 12 chapters and a summary. It deals with the philosophical questions of model building first, followed by applications to business and economics. Investment, sequenced divisions, decision and utility theory and competitive problems are some of the subjects to which individual chapters are devoted.

Roberts (1976) This book deals mainly with two types of formulations - graph theoretic and Markov chains, and their use in modelling a range of topics in social and biological sciences. This is an excellent book for the use of graph theoretic representations in system characterization. The approach is mainly axiomatic and the emphasis is on analytical methods.

Ross (1983) This book discusses various stochastic dynamic formulations and their use in modelling. In particular, it examines Markov chains, Poisson processes, and renewal theory. The application of these to queues and reliability are discussed. The final chapter discusses parameter estimation for some of the formulations.

Saaty (1973) This book consists of the notes used at a summer seminar on mathematical modelling. The notes are divided into three parts. Part I is a general discussion of mathematics and behavioural sciences with emphasis on model planning and building and the process of decision making. Part II

investigates eight topics central to mathematical modelling of social sciences: allocation and optimization, conflict resolution, scheduling tasks to machines, flow and synthesis problems in networks, inventory control, queues and congestions, reliability, maintenance and renewals, and search. Part III describes some structured and unstructured problems. Among these are the travelling salesman problem, arborescences and questionnaires, epidemics and stochastic barriers, and parking at an aircraft terminal.

Saaty and Alexander (1981) This book is divided into three parts. Part 1 deals with methodology; Part 2 with the "framework"; and Part 3 with applications. The different types of formulations considered in the book are given in Part 2. Each formulation is illustrated by a simple application involving the formulation. The chapter entitled "Equations" deals with different types of equation formulations, and the chapter entitled "Stochastic processes" looks at a range of stochastic formulations. The applications cover a wide range of topics and the emphasis is on model building and analysis.

Sheep (1983) This is the 27th volume of the *Proceedings of Symposia in Applied Mathematics*. The subject covered, computed tomography, is discussed in seven papers. Each paper suggests problems, both relevant and of "intrinsic interest" to mathematicians. The volume addresses the mathematical modelling problem of finding the appropriate level of abstraction in a mathematical model of a real-world situation.

Spriet and Vansteenkiste (1982) This book examines the use of stochastic difference equation formulations and deterministic partial differential equation formulation. Parameter estimation is discussed in great detail for stochastic difference equations. The numerical solutions of partial differential equations are discussed, along with software packages. The application of partial differential equations to environmental problems is discussed briefly. In addition, there is a chapter on hardware trends and their impact on simulation.

Weinberg (1975) This is an introductory book which assumes a knowledge of high school algebra. The book is divided into seven chapters, each of which ends with a number of exercises. The book also includes an appendix on how to read mathematical notation. The chapters are entitled: the problem, the approach, system and illusion, interpreting observations, breaking down observations, describing behaviour, and some systems questions.

Zeigler (1976) This book concentrates on developing a theory of modelling and simulation. The system characterization is done with the aim of stimulating the model on a computer. Various aspects of simulation are

discussed in great detail. Appendix A deals with a case study – Modelling the human brain.

Zierep (1971) This book discusses dimensional analysis, similarity laws, and dimensionless parameters. It uses the study of classical mechanical and thermodynamic similarity laws of gas dynamics to cover subjects such as linearized subsonic and supersonic flow, transonic and hypersonic flow, and a brief survey of corresponding flows with relaxation.

2.3 Publication Details

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3 Models, Modelling and Teaching Modelling*

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*IJMEST = International Journal of Mathematics Education in Science and Technology;
IMA = Institute of Mathematical Applications.

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4 Journals

4.1 Journals on Mathematical Modelling

- [1] *Mathematical and Computer Modelling*
- [2] *Applied Mathematical Modelling*
- [3] *International Journal of Modelling and Simulation*
- [4] *Journal of Interdisciplinary Modelling and Simulation*
- [5] *Stochastic Models*

The following journals contain many articles on models and modelling.

- [6] *Teaching Mathematics and its Applications*
- [7] *Bulletin of the Institute of Mathematics and its Applications*
- [8] *UMAP Journal: The Journal of Undergraduate Mathematics and its Applications*

UMAP modules contain many articles on models and modelling.

4.2 Abstracting and Indexing Journals

It is impossible to give a complete list of abstract and indexing journals as it would run into several hundred. Instead, we give a short list which covers nearly all the disciplines where mathematical models have been used for solving problems.

- [1] *Mathematical Reviews*
- [2] *Statistical Theory and Method Abstracts*
- [3] *Biological Abstracts*
- [4] *Applied Ecology Abstracts*
- [5] *Ecology Abstracts*
- [8] *Population Abstracts*
- [9] *Entomology Abstracts*
- [10] *Pollution Review*
- [11] *Forestry Abstracts*
- [12] *Aquatic Sciences and Fisheries Abstracts*
- [13] *Tropical Diseases Bulletin*
- [14] *Population Index*
- [15] *Geo Abstracts*
- [16] *Sociological Abstracts*
- [17] *Business Periodicals Index*
- [18] *Index of Economic Articles*
- [19] *International Bibliography of Economics*
- [20] *Computer and Control Abstracts*
- [21] *Computing Reviews*
- [22] *The Engineering Index*
- [23] *Applied Mechanics Reviews*
- [24] *Cybernetics Abstracts*
- [25] *International Abstracts in Operations Research*
- [26] *Physics Abstracts*
- [27] *British Chemical and Physiological Abstracts*
- [28] *Psychological Abstracts*
- [29] *A London Bibliography of the Social Sciences*
- [30] *International Political Science Abstracts*
- [31] *Linguistic and Language Behaviour Abstracts*
- [32] *Bibliographie Linguistique*
- [33] *Bibliographie Geographique Internationale*
- [34] *Education Index*
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- [36] *International Bibliography of the Social Sciences*

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